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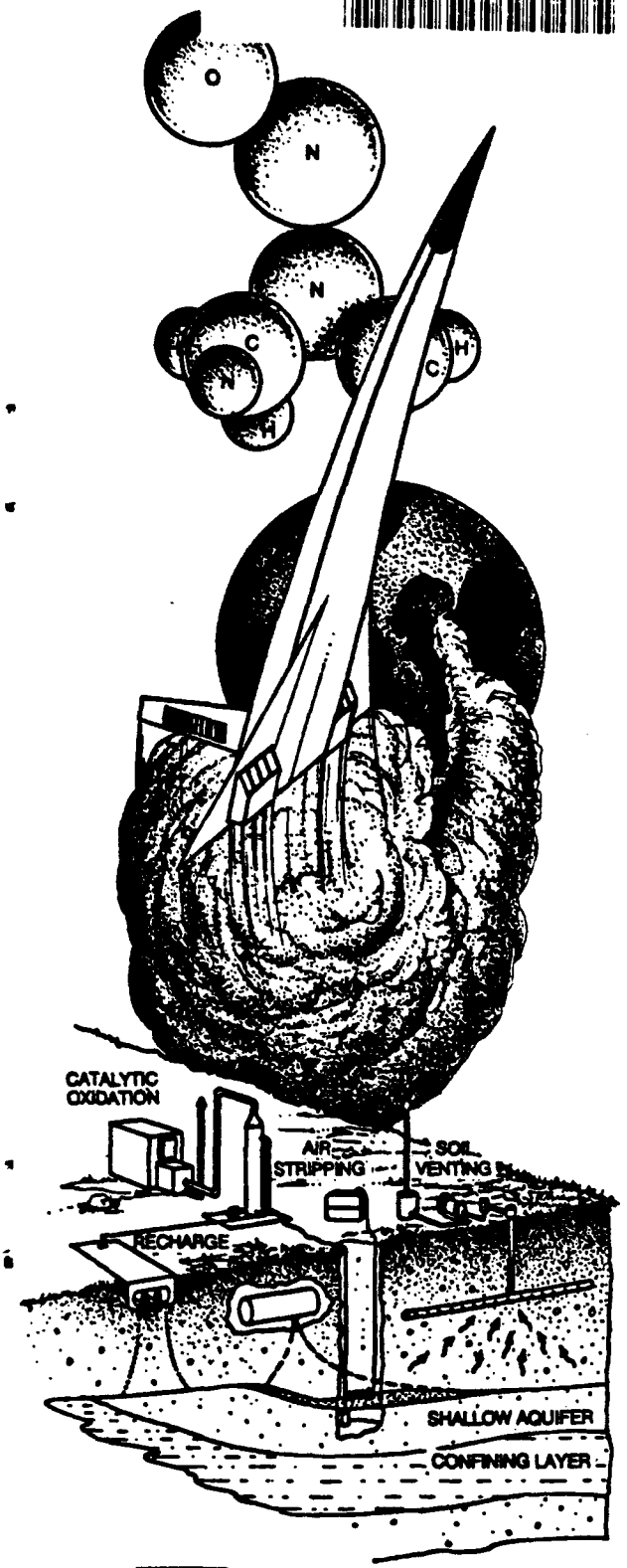

SPECTROSCOPIC STUDIES OF HAZARDOUS FUEL INTER-ACTIONS WITH SOILS

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AIR FORCE ENGINEERING AND SERVICES CENTER
HQ AFESC/RDVC
TYNDALL AFB FL 32403-6001

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This report describes the development and application of techniques for the spectroscopic study of hazardous fuel compounds in soils. The objective is to obtain improved models of bulk pollutant transport through soils. Two approaches have been used for this study: one consists of in-situ measurements of electronic and vibrational interactions via ultraviolet-visible spectroscopy and infrared spectroscopy, respectively; the other incorporates analytical separation techniques to extract contaminants from soils and identify individual reaction products. Initially, montmorillonite clay has been chosen as a prototype soil sample because the structure of this clay is well characterized and spectroscopic results can be readily interpreted. Further simplification has been obtained by exposing the clay samples to individual fuel components rather than mixtures. An interpretation of one clay/fuel system has been accomplished. The plan is to gradually increase the complexity of the samples until typical field conditions can be modeled.

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EXECUTIVE SUMMARY

A. OBJECTIVE: Determine the fate of aromatic fuel compounds in soils via molecular-level measurements, and thereby obtain improved models of bulk pollutant transport through soils. These models would enhance the ability of the Air Force to contain and clean up fuel spills.

B. BACKGROUND: Current models of pollutant transport through soils are based entirely on bulk measurements (e.g. grams of chemical sorbed per gram of soil). These models effectively describe pollutant transport in some systems, but they cannot be reliably extrapolated to new systems unless they are founded on correct molecular-level assumptions.

C. SCOPE: A study was conducted on electronic and vibrational interactions of fuel compounds with montmorillonite clay. Montmorillonite was chosen as a prototype soil sample because the structure of this clay is well characterized and spectroscopic results can be readily interpreted. Further simplification was obtained by exposing clays to individual fuel components rather than mixtures. Both physical and chemical changes of montmorillonite were monitored as contamination proceeded in a controlled environment. Analytical separation techniques were used to extract contaminants from the montmorillonite samples and to identify individual reaction products.

D. METHODOLOGY: Ultraviolet-visible and infrared spectroscopy were used to obtain electronic and vibrational information, respectively. The former measures electronic properties of molecules, particularly the transformation of neutral organic molecules in soils to ions. The latter measures chemical changes via changes in molecular vibrations.

Extractions of clays were performed by repeatedly exposing the clays to common solvents such as acetone and chloroform. Separation of reaction products was effected by gas chromatography. Reaction products were than identified using either infrared spectroscopy or mass spectroscopy in conjunction with spectral library searches.

E. TEST DESCRIPTION: Some tests were conducted in a controlled-environment cell containing a self-supporting clay film (which was thin enough to transmit light), a vapor-phase aromatic contaminant, and a desiccant. This setup enabled clay/pollutant interactions to be studied as a function of relative humidity. The cell was transported back and forth between an ultraviolet-visible spectrometer and an infrared spectrometer to obtain tandem measurements of the clay at various stages of desiccation.

Other tests were conducted using a reflux apparatus containing about 1 gram of clay and about 70 mL of a pure liquid contaminant. The clay was refluxed overnight and then extracted in a commercial Soxhlet extraction apparatus. The extract was separated into its constituent compounds via a commercial gas chromatograph and analyzed with either a mass spectrometer or a Fourier transform infrared spectrometer.

F. RESULTS: A characterization of a simple system was accomplished: that of para-dimethoxybenzene on montmorillonite. This system was chosen as a starting point because the spectroscopic results could be readily interpreted and, therefore, the techniques for studying this system could be efficiently developed.

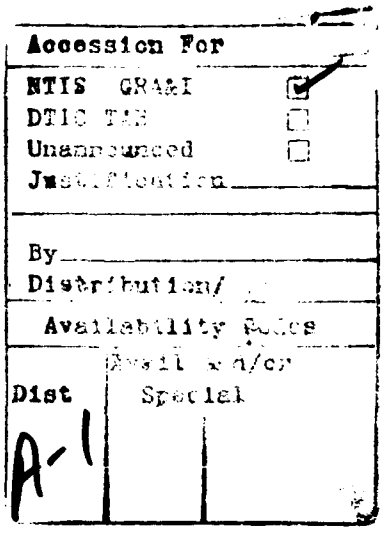
G. CONCLUSIONS: An initial step has been taken toward understanding the behavior of fuel contaminants in soils. Once some simple clay/pollutant systems have been interpreted, it should be possible to predict the behavior of similar systems. The

complexity of the systems will then be increased to a level representative of that existing at Air Force fuel facilities.

Parallel studies are underway at the University of Florida using a variety of techniques that cannot readily be implemented at Tyndall AFB. Complementary studies of bulk transport of pollutants through soils are in progress at Tyndall AFB. This multifaceted approach should improve the ability of the Air Force to minimize the environmental impact of fuel spills.

H. RECOMMENDATIONS: Future research should be directed towards increasing the complexity of the contaminated soil systems to a level comparable to field samples. This will likely require the implementation of the supercritical fluid extraction technique since conventional solvent extractions have been found to be of limited usefulness in removing pollutants from clays.

Studies on contaminated clays might lead to the development of an artificially modified clay that efficiently traps any aromatic molecules that sorb onto it. Such a clay could be used to contain a fuel spill within a localized area.



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PREFACE

This report was prepared by the Engineering and Services Laboratory of the Air Force Engineering and Services Center (AFESC), Tyndall Air Force Base FL 32403-6001. This work was sponsored by AFESC. Dr. Terence L. Tipton and Dr. Daniel A. Stone (AFESC/RDVC) were the government project officers. This report summarizes work accomplished between October 1989 and October 1990 under program element 61101F.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public including foreign nationals.

This technical report has been reviewed and is approved for publication.

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SECTION I

INTRODUCTION

A. OBJECTIVE

The objective of this project is to determine the mechanisms by which component compounds of Air Force fuels interact with soils, and thereby improve the predictive capabilities of macroscopic models of pollutant transport through soils. Current models of soil transport (e.g. see Reference 1) are derived from bulk measurements and lack a firm theoretical foundation based on molecular-level interactions.

B. BACKGROUND

This project is an in-house study in progress at Tyndall AFB under the category of Environmental Impact Assessment. Its purpose is to provide additional framework for concurrent in-house studies of bulk transport properties of aquifer pollutants. It is being supported by parallel research underway at the Soil Science Department of the University of Florida (UF) under a contract with the Air Force. The UF provides additional instrumentation and expertise necessitated by the complex nature of this project.

A number of different types of measurements are required to understand the nature of interactions of pollutants with soils. These can be divided into two categories: (1) those that are

performed directly on the soils; and (2) those that are performed on materials extracted from the soils. The former includes Fourier transform infrared (FT-IR) spectroscopy, ultraviolet-visible (UV-VIS) spectroscopy, and gravimetric measurements. The latter includes the combination of gas chromatography and mass spectrometry (GC/MS); and the combination of GC, matrix-isolation (MI), and FT-IR spectroscopy (GC/MI/FTIR).

Many of the above measurements can be made with equipment available at Tyndall AFB. Important supplemental information can be obtained from the wider range of facilities available at UF. This includes: (1) x-ray diffraction to monitor changes in interlayer spacing of soils that occurs on adsorption of fuel compounds; (2) MI spectroscopy of ions to probe the behavior of organic ions that form in soils; and (3) FT-Raman spectroscopy to selectively excite a specific molecular specie in a soil from among the many species that are likely to be present.

One approach that has been developed for studying polluted soil samples is to combine the techniques of UV-VIS and FT-IR spectroscopy. UV-VIS spectroscopy measures electronic properties of molecules, particularly the transformation of neutral organic molecules in soils to ions. FT-IR spectroscopy measures chemical changes via changes in molecular vibrations.

Spectroscopic absorption can be related to macroscopic properties by recording spectroscopic and gravimetric data simultaneously. A microbalance provides the sensitivity necessary

to measure sorption of pollutants onto the tiny quantities of sample that are used in spectroscopic measurements.

Initially, clays are being used as prototype soil samples because they: (1) have structures that are well characterized; (2) can be fashioned into self-supporting films that can be examined via conventional spectroscopic absorption measurements; (3) readily sorb atmospheric moisture, and are thus amenable to the study of reaction rate versus humidity; (4) have large interlayer surface areas that enable a relatively large quantity of contaminant sorption per gram of clay; and (5) are important components of natural soils.

In-situ measurements on clays have proven to be useful for the study of reactions on clay films, but these measurements are deficient in two areas. First, soils are opaque except when examined in very minute quantities. Consequently, the sensitivity of spectroscopic measurements is very limited. Second, reaction products are difficult to identify when several are simultaneously present in a soil sample. These deficiencies can be at least partially remedied by extracting soil samples with nonaromatic solvents such as chloroform and acetone. Reaction products can then be separated using standard analytical techniques, particularly GC. Identification of products can be achieved by introducing the effluent of a GC to either a mass spectrometer or an FT-IR spectrometer.

In addition to standard solvent extraction, supercritical fluid extraction (SFE) may be applicable to contaminated soils.

A supercritical fluid is a highly compressed gas whose temperature is too high to permit condensation to a liquid. Supercritical fluids are often highly effective solvents for extracting solutes from solid samples, since these fluids can easily penetrate microporous materials.

It is well known that aromatic molecules are susceptible to ionization when they are absorbed into the interlayers of clays (e.g., see Reference 2). Such ionization is induced by transition metal ions which occur naturally in the interlayers. Formation of aromatic ions is evidenced by color changes that are readily discernible to the naked eye. The aromatic ions often polymerize, particularly under dry conditions. An understanding of the reaction mechanisms has been achieved only for some very simple systems (e.g., see Reference 3). Accurate modeling of the behavior of pollutants in a natural soil environment will require much additional study.

C. SCOPE

Section II of this report begins with a procedure for preparing clay film samples for spectroscopic analyses. Next, it explains how contaminated clays are extracted for analyses of reaction products. Third, it describes the instrumentation used for examining clays and clay extracts.

Section III presents some of the results obtained by applying the experimental procedures of Section II. It includes a

description of tandem FT-IR/UV-VIS experiments on clays contaminated with components of Air Force fuels. It also includes results of extraction studies via GC/MS.

Section IV presents conclusions obtained from preliminary data, and Section V suggests how these results may be extended in the future.

The Appendix tabulates computer programs that were written to collect, organize, and plot data on the computer work stations for the FT-IR and UV-VIS spectrometers.

SECTION II

EXPERIMENTAL PROCEDURES

A. CLAY FILM PREPARATION

1. Starting Material

The starting material for all experiments was SAz-1 montmorillonite obtained from the Clay Minerals Society Source Clay Minerals Repository of the University of Missouri.

2. Size Fractionation

The starting material had to be size fractionated to obtain a pure clay. The procedure for this process is as follows:

a. Mix 30.0 grams of SAz-1 montmorillonite with 1.20 liters of 0.5 M NaCl to form a suspension. The NaCl facilitates the size-fractionation of the clay (described in Step h).

b. Distribute the suspension equally among six 250-mL centrifuge bottles.

c. Centrifuge the bottles at 3000 rpm for 10 minutes.

d. Decant and discard the supernatant from the bottles.

e. Add 200 mL of distilled deionized water to each bottle.

f. Shake the bottles in a commercial shaker at about 2000 vibrations per minute until uniform suspensions are obtained (typically 10 minutes).

g. Repeat the above washing procedure (Steps c-f) until the addition of silver nitrate solution to the wash gives no precipitate (typically, five washings are required). Increase the centrifuging times if any of the clay remains suspended after completion of Step c.

h. Remove the coarsest particles from the suspensions by centrifuging the bottles for a few minutes or by letting the suspensions sit undisturbed for approximately 30 minutes.

i. Decant the bottles and save only the decanted material.

j. Centrifuge the bottles at 3000 rpm for 10 minutes.

k. Decant and discard the supernatant from the bottles.

3. Ion Exchange

The clay samples were subjected to ion exchange to replace the ions which were naturally present in the clay with the ions which were targeted for study. The following procedure describes how Cu-exchanged montmorillonite is produced from the product of the size-fractionation procedure outlined above:

a. Add 200 mL of 0.05 M Cu(II)-chloride to each of the bottles.

b. Shake the bottles at 2000 vibrations per minute until uniform suspensions are obtained.

c. Centrifuge the bottles at 3000 rpm for 10 minutes.

d. Decant and discard the supernatants from the bottles.

e. Repeat Steps a-b.

f. Perform the washing procedure (Steps c-f of the size fractionation procedure) until the addition of silver nitrate solution to the wash gives no precipitate.

4. Production of Clay Films

a. Determine the approximate mg clay per mL of suspension by weighing a sample of the suspension before and after drying it. (Note: For the SAz-1 montmorillonite used in this report, yields of better than 50 percent were recorded for the size-fractionation step).

b. Dilute the clay suspension with distilled deionized water to obtain roughly 2 mg of clay per mL of suspension. If the concentration is too low, a self-supporting film cannot be produced. If the concentration is too high, the resulting film will absorb too much light to be useful for spectroscopic measurements.

c. Using a pipet, deposit several 1 mL samples of the final clay suspension onto a polyethylene sheet. Allow 18 hr for the samples to dry in the open air. If faster drying is needed, put the polyethylene sheet in a box equipped for a dry air flow.

d. Peel the dried clay samples from the polyethylene sheet by running the sheet over a knife edge. The dried clay films are pale green, roughly circular, and about 1.5 cm in diameter.

B. COMMERCIAL INSTRUMENTATION

The infrared measurements described in this report were recorded on a Nicolet Model 740 FT-IR spectrometer equipped with an HgCdTe-A detector (5000 to 600 cm^{-1}). The resolution was set at 0.5 cm^{-1} for MI experiments, and 2.0 cm^{-1} for all other experiments. The iris aperture for the source radiation was set at 2 mm. At least 100 averaged scans were recorded for each spectrum.

UV-VIS spectra were recorded on a Perkin-Elmer Model 3840 photodiode-array spectrophotometer at 1.5 nm resolution. Each spectrum consisted of 256 averaged scans covering the range from 190 nm to 900 nm.

GC/MS spectra were recorded on a Hewlett-Packard Model 5980A GC, coupled to a Model 5970 mass selective detector. A 1.0 microliter sample was injected via the splitless mode into a 30-meter long, 0.322 mm i.d. capillary coated with a 5 percent phenyl, 95 percent methyl, 0.25 micrometer polymethylsiloxane film (J&W Scientific). The oven was held at 40°C for 4 minutes, ramped to 250°C at 10°C $minute^{-1}$, and held at 250°C for 20 minutes. The carrier gas was helium, and the column head pressure was 15 psi above atmospheric pressure.

C. CLAY-FILM CELL FOR TANDEM FT-IR AND UV-VISIBLE STUDIES

A controlled-environment cell was constructed to permit analyses of clay films via tandem FT-IR and UV-VIS measurements. A 25 mm i.d. KF® tee was augmented with two additional arms to produce a cross having four horizontal arms and one vertical arm (Figure 1). This configuration enabled a pair of infrared transmission windows (KCl) and a pair of UV-VIS transmission windows (sapphire) to be mounted on the horizonal arms of the cell at the same time. The vertical arm was used to suspend a rotatable stainless steel sample holder in the path of either the FT-IR or UV-VIS beam. The extra horizontal arm was made shorter than the other arms to permit the cell to fit into the 5-inch wide sample compartment of the Perkin-Elmer UV-VIS spectrometer. Two 0.25-inch i.d. stainless steel tubes were silver-brazed onto opposing arms of the cell to permit purging of the cell with dry air (dew point < -75°C). The cell length was 5.6 inches for the infrared path, and 4.8 inches for the UV-VIS path. The clay-film holder consisted of either 3/8-inch or 1/2-inch i.d. stainless steel washers. The 3/8-inch size was the minimum that could readily accommodate the 1/8-inch by 1/4-inch (horizontal by vertical) rectangular UV-VIS beam.

The above cell was used to record the chemisorption of an aromatic compound onto a clay film as a function of humidity. A few tenths of a gram of a pure aromatic compound were added to the

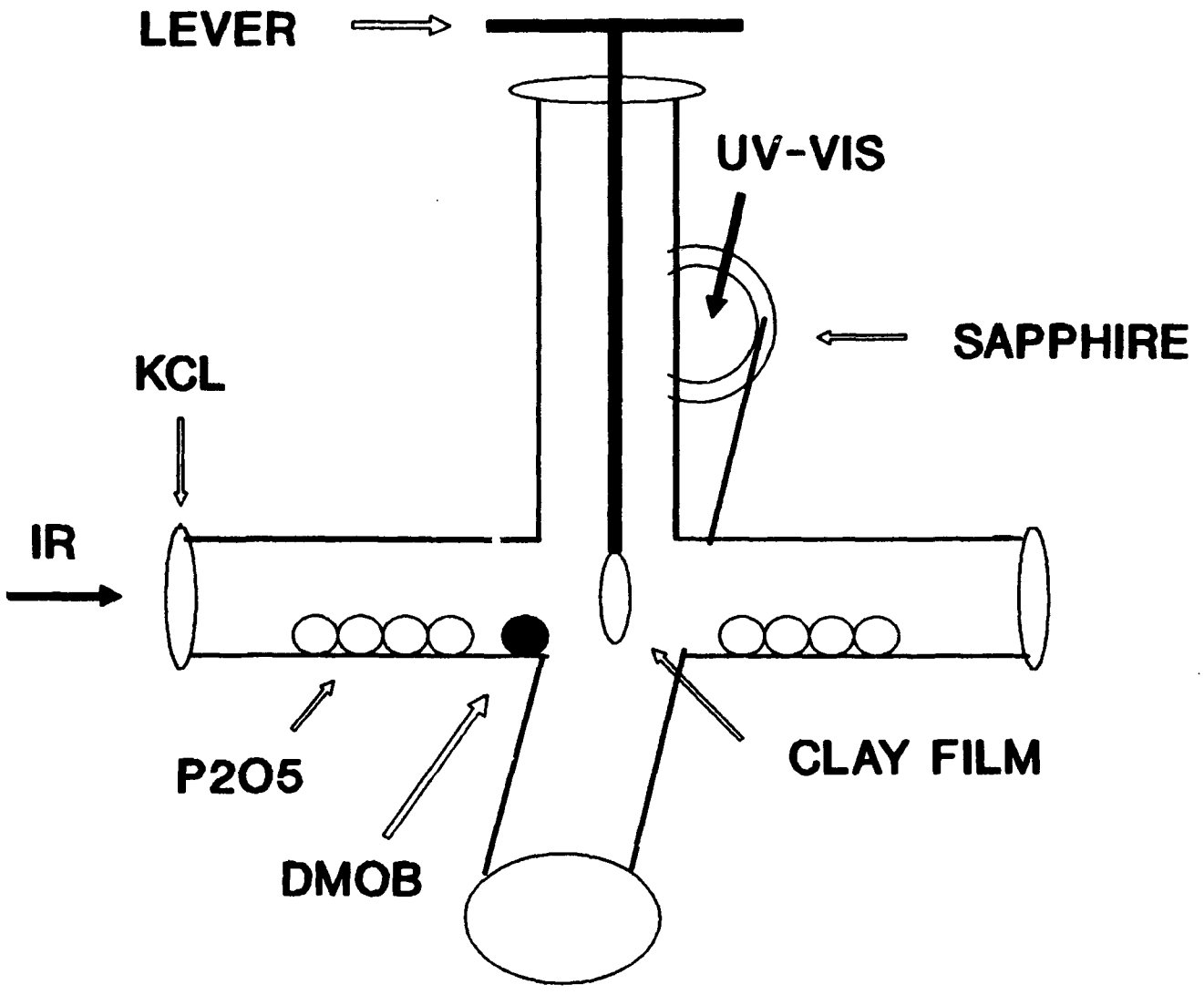

Figure 1. Clay-Film Cell for Tandem FT-IR and UV-VIS Experiments.

cell at the start of an experiment along with P_2O_5 desiccant. The aromatic compound was placed in the center of the cell, and the desiccant was placed immediately next to it in all four horizontal arms. This operation was carried out in a glove bag of dry air to protect the desiccant from atmospheric moisture. A clay film was introduced to the cell within the next several minutes. This caused the clay film to gradually dry over a period of several hours. The removal of water from the clay was typically accompanied by the chemisorption of the aromatic compound onto the clay from the vapor phase.

A clay film was formed by pipetting 1 mL of a 2 mg/mL clay suspension onto a polyethylene sheet. The area of the dried film was typically 2 cm^2, resulting in a 1 mg cm^{-2} density. Since the infrared beam had a diameter of 0.2 cm, the mass of the clay that was exposed to the infrared beam was about 30 ng. The corresponding mass for the UV-VIS beam was about 200 ng.

D. CLAY EXTRACTION

1. Sample Preparation

An aliquot of the stock clay suspension obtained via the clay preparation procedure of Section II-A was placed in a mortar and heated until all of the water was vaporized. Typically, 0.5 grams of dehydrated clay was used for extractions. The clay was ground into a fine powder with a mortar and pestle, transferred to

a modified 100 mL round-bottom (RB) flask, and refluxed overnight (about 16 hr) in 70 mL of a liquid aromatic contaminant under a nitrogen atmosphere (Figure 2). The RB flask was outfitted with a gas inlet tube and Teflon® valve to permit the nitrogen to purge the apparatus prior to the start of refluxing. After this initial purge, the Teflon® valve was shut off, and the nitrogen inlet tube was transferred to the top of the condenser to minimize loss of the refluxing fluid.

After the refluxing was finished, the clay was separated from the solvent either by filtration or by decanting the RB flask and vaporizing the remaining liquid. The clay residue was then subjected to the Soxhlet extraction procedure given below.

2. Soxhlet Extraction

Soxhlet extraction is a method whereby a sample mixture is repeatedly exposed to a pure recycled solvent to enable even barely soluble components of the sample to be collected. A schematic diagram of a Soxhlet extractor is shown in Figure 3. The solvent is placed in a heated round-bottom (RB) flask, and a sample is placed in a cellulose thimble in the upper compartment. The solvent vaporizes from the RB flask, flows up to a condenser, and drips down into the upper compartment. When the upper compartment becomes full, the liquid siphons back into the RB flask. This process repeats indefinitely, causing extracted solute to accumulate in the RB flask.

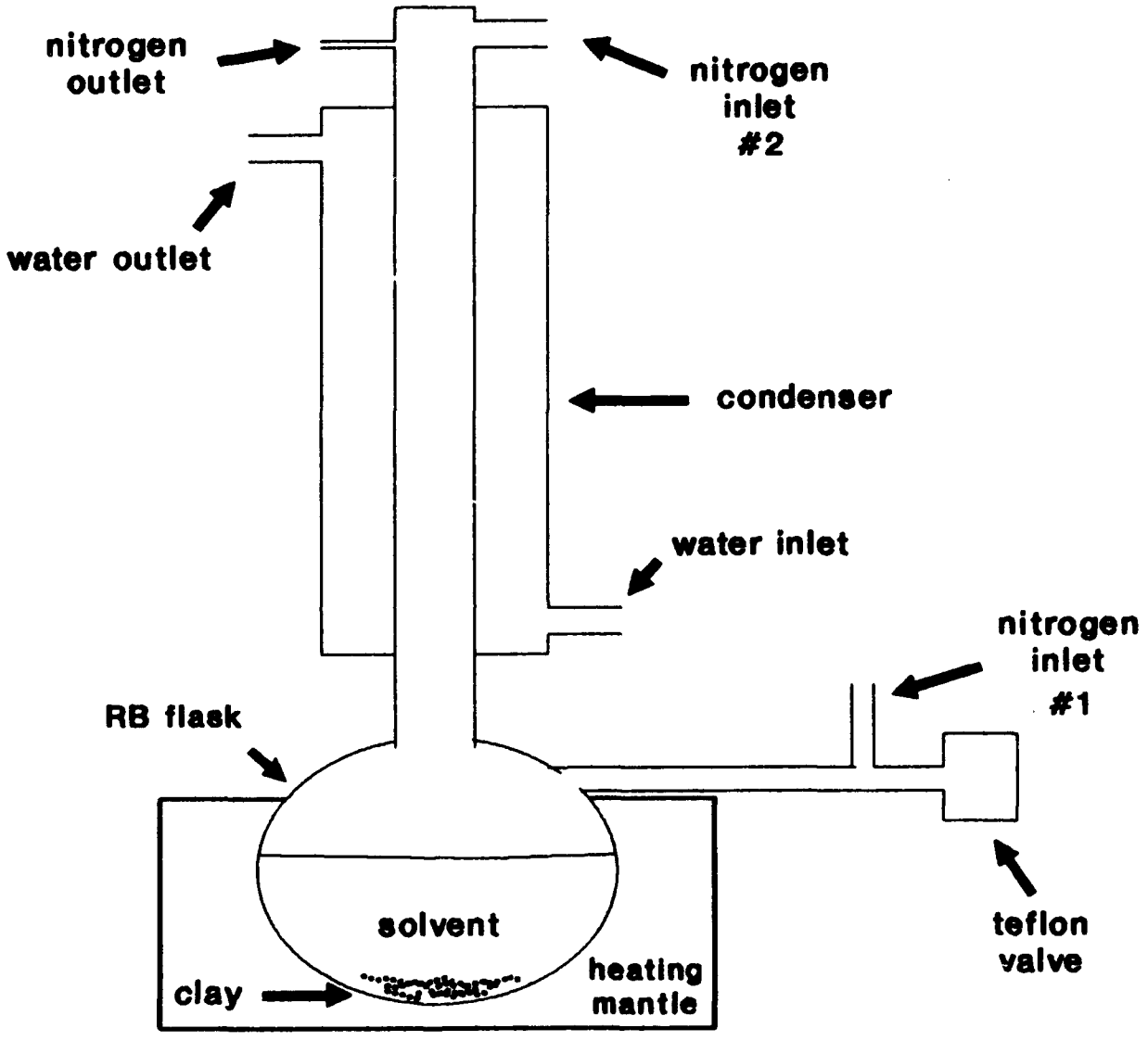

Figure 2. Apparatus for Refluxing Clay Under Nitrogen.

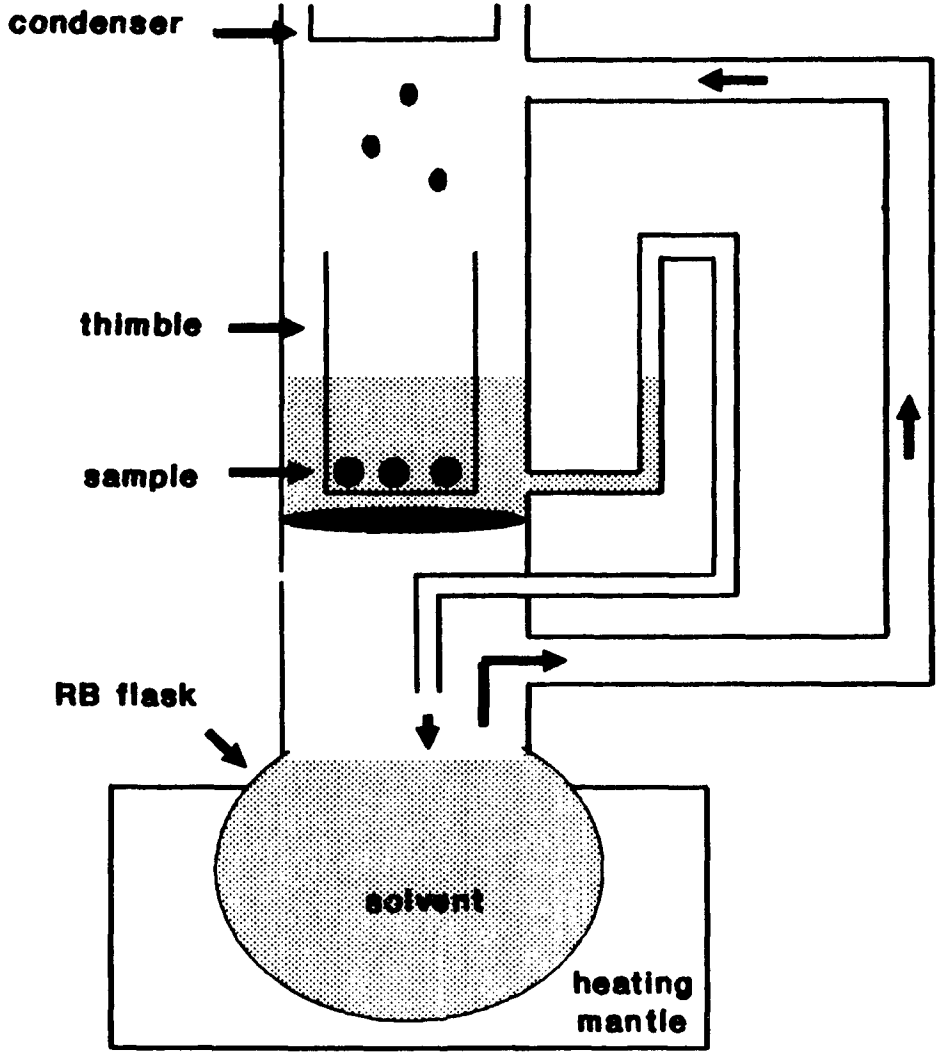

Figure 3. Soxhlet Extractor.

The above procedure was applied to numerous samples of montmorillonite powder containing adsorbed fuel components. Usually, several solvents had to be used on a given sample because no single solvent could extract all of the reaction products.

3. Supercritical Fluid Extraction

Supercritical fluid extraction (SFE) is a method whereby a highly compressed gas (typically 100 atm), whose temperature is too high to permit condensation, is used to extract components from a solid sample (Reference 4). SFE is often more effective than conventional extraction techniques because supercritical fluids can penetrate into microporous materials more readily than liquids can. Carbon dioxide is usually used as the solvent for SFE because of its general effectiveness and its relatively low supercritical temperature (31°C) and pressure (73 atm).

A simple SFE apparatus has been designed for testing the effectiveness of the SFE technique on contaminated clays (Figure 4). A pump is required in this system since commercial cylinders of carbon dioxide are not pressurized as high as the 73 atm minimum pressure required to produce a supercritical fluid state. The sample container and gas transfer tubes must be heated with an oven or heating tape (not shown) to achieve the requisite 31°C temperature. The sample container is a stainless steel cylinder with a lid. Bolts are used to press the lid down on an o-ring to produce a high-pressure seal.

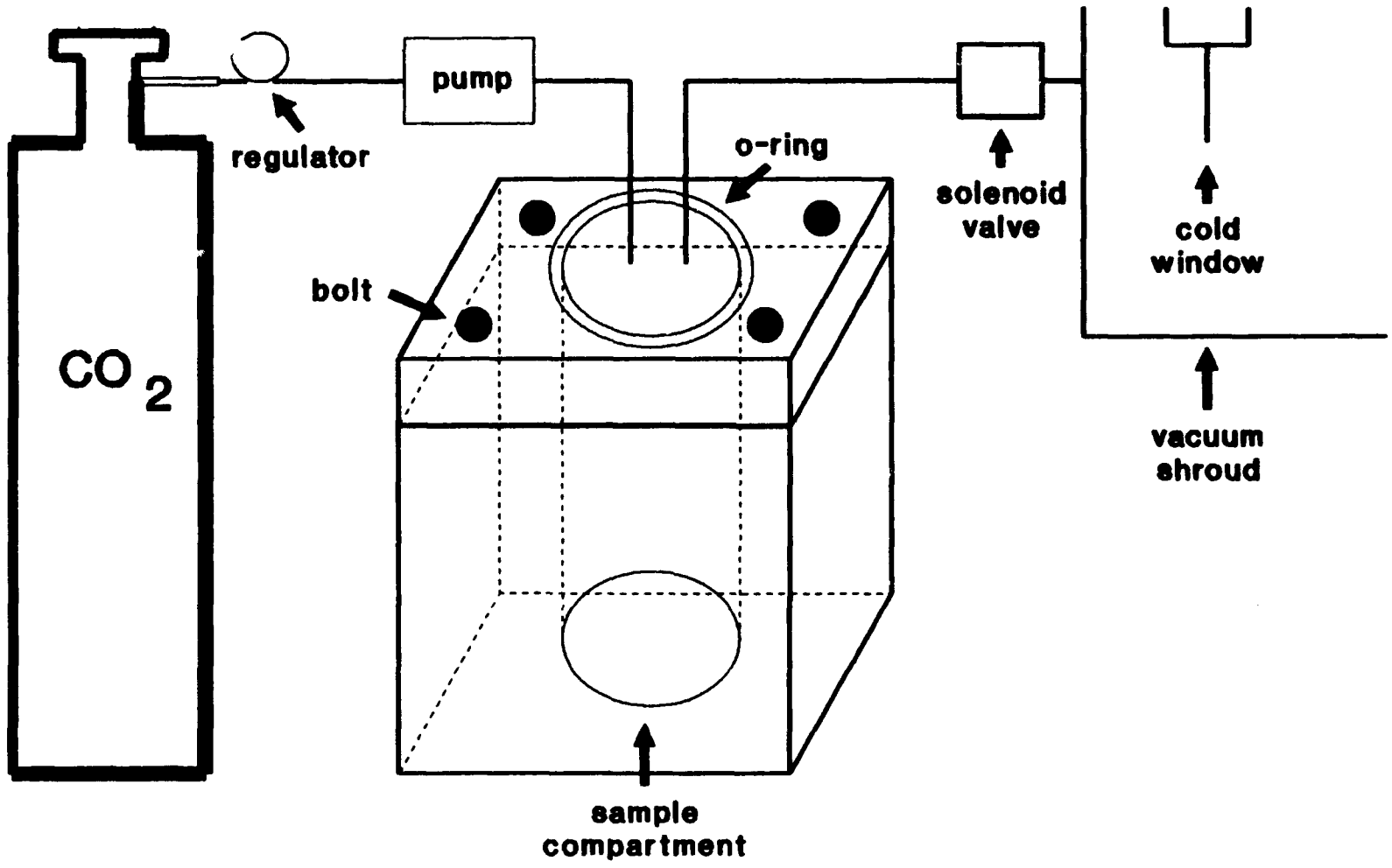

Figure 4. Apparatus for Matrix Isolation of Supercritical Fluid Extracts.

The effluent from the above apparatus is condensed onto a cryogenically cooled mirror to isolate the extract in a carbon dioxide lattice. A pulsed solenoid valve limits the rate at which the effluent emerges from the outlet. This scheme does not enable the extracted material to be separated into its component substances but it will determine whether SFE is effective in removing sorbed substances from contaminated clays.

4. Sample Heater for Matrix Isolation

A sample heater was constructed for the MI apparatus to: (1) test whether simple distillation of clay extracts would effectively separate component compounds; and (2) provide a means of obtaining reference MI spectra for compounds with low vapor pressures.

The heater (Figure 5) consisted of two 1000-ohm enamel wirewound power resistors connected in parallel to a variable transformer. A temperature of 335°C was observed when this heater was operated in ambient air at 136 volts. In normal use, the heater was interfaced with the shroud of the expander module of a closed-cycle refrigerator (Air Products Displex Model CSA-202), and was operated in a vacuum.

The sample material was placed at the end of a 5/16-inch o.d. stainless steel tube which fitted snugly inside of the hollow cores of the power resistors. The end of this tube contained a removable insert constructed from a 1/4-inch i.d. Swagelok®

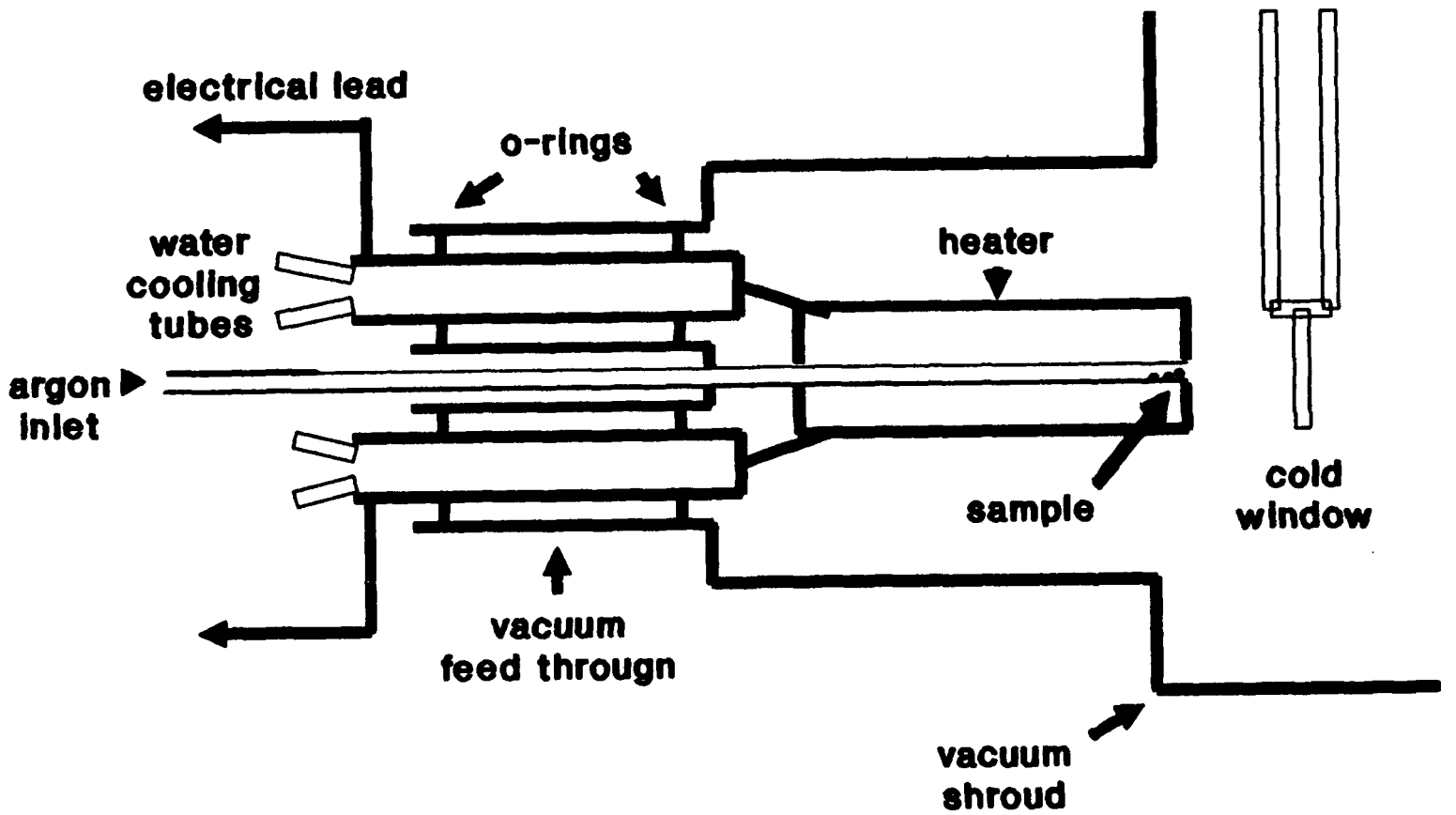

Figure 5. Sample Heater for Matrix-Isolation Experiments.

ferrule soldered to a circular piece of stainless steel foil with a pinhole in it. This insert allowed a sample to be easily placed into the core of the heater and prevented the sample from being sucked out of the tube during evacuation.

The heater was located within a cylindrical cooling jacket constructed from concentric 1-5/8-inch o.d. and 1-1/8-inch o.d. copper tubes, 4-1/2-inches long. One end of this jacket was silver-brazed to a 1-3/4-inch square stainless steel flange with a 1-inch entrance hole in it; the other end was silver-brazed to a flange through which the sample tube and two electrical feed-throughs passed. The feed-throughs consisted of concentric 1/4-inch and 3/8-inch o.d. stainless steel tubes separated by two pairs of #007 Viton® o-rings. Both tubes were filed on a lathe to create enough space for the o-rings to fit between them. Each o-ring was held in place by a pair of 1/4 inch i.d. Swagelock® ferrules which were silver-brazed into position and filed so that their outer diameters were smaller than the outer diameters of the o-rings. The electrical current passed through the 1/4-inch stainless steel tubes and through short pieces of copper wire to the power resistors. These tubes were cooled by transporting water in and out of them via two 1/8-inch o.d. stainless steel tubes. Originally, the feed-throughs were designed so that the cooling water passed between the 1/4-inch and 3/8-inch stainless steel tubes but this scheme was abandoned after failure of an o-ring enabled cooling water to leak directly into the evacuated shroud.

A thoroughly dry sample tube was essential to the effectiveness of the heater since a moist tube resulted in highly absorbing ice bands which obscured a large part of the most useful regions of the infrared spectrum. The tube was dried, while empty, by heating it under a vacuum at the maximum temperature to be used for the sample. The dryness was maintained during the insertion of the sample by flowing a dry vapor through the tube.

One deficiency of the above heater was that it contained exposed areas of relatively high voltage, and was thus vulnerable to catastrophic short circuits. This deficiency will be minimized by replacing the 1000-ohm power resistors with 2-ohm resistors as soon as the latter become available. The smaller resistors will be safer because they will be operated at much lower voltages than those presently required for the larger resistors.

5. Apparatus for: Gas Chromatography / Matrix Isolation / FT-IR Spectroscopy

The matrix-isolation (MI) apparatus used in conjunction with the current study on clays is largely the same as described in a previous technical report (Reference 5). A cryogenic refrigerator freezes a sample material within a lattice of an inert solvent such as argon. The sample molecules are thereby isolated at a density similar to that of a vapor, but without the rotational motion of the vapor state. The absence of rotational structure in

the infrared spectrum simplifies assignments of vibrational bands and facilitates identification of the absorbing specie.

Infrared reference spectra for pure compounds are obtained by spraying a gaseous sample/argon mixture onto an infrared transmission window. A similar procedure can be used for analyzing the effluent of a gas chromatograph (Reference 6). Such a scheme is useful for the identification of reaction products extracted from contaminated clay samples.

To implement the GC/MI/FTIR method, it is necessary to calculate the sensitivity needed to detect solutes eluted from a gas chromatograph with an infrared detector. The quantity of solution used for GC analysis is typically 1 microliter, or roughly 1 mg. A typical quantity of sample needed to produce an optimum infrared spectrum is about 30 ng, assuming that the sample diameter and beam diameter are both about 2 mm. Thus a solute/solvent mass ratio of 1:30 should produce a strong solute spectrum, and a much less favorable ratio may still be adequate to enable a compound to be detected and identified.

The sample diameter limitation of 2 mm has significant consequences in the design of a GC/MI/FTIR experiment. First, the tip of the GC column must be placed roughly 1 mm from the substrate. Transmission windows are unsuitable under these circumstances because they have insufficient heat conductivity to freeze the argon carrier gas at the required rate. Therefore, a gold-coated copper mirror (M1 in Figure 6) was used instead. Additional mirrors were used in conjunction with the copper mirror

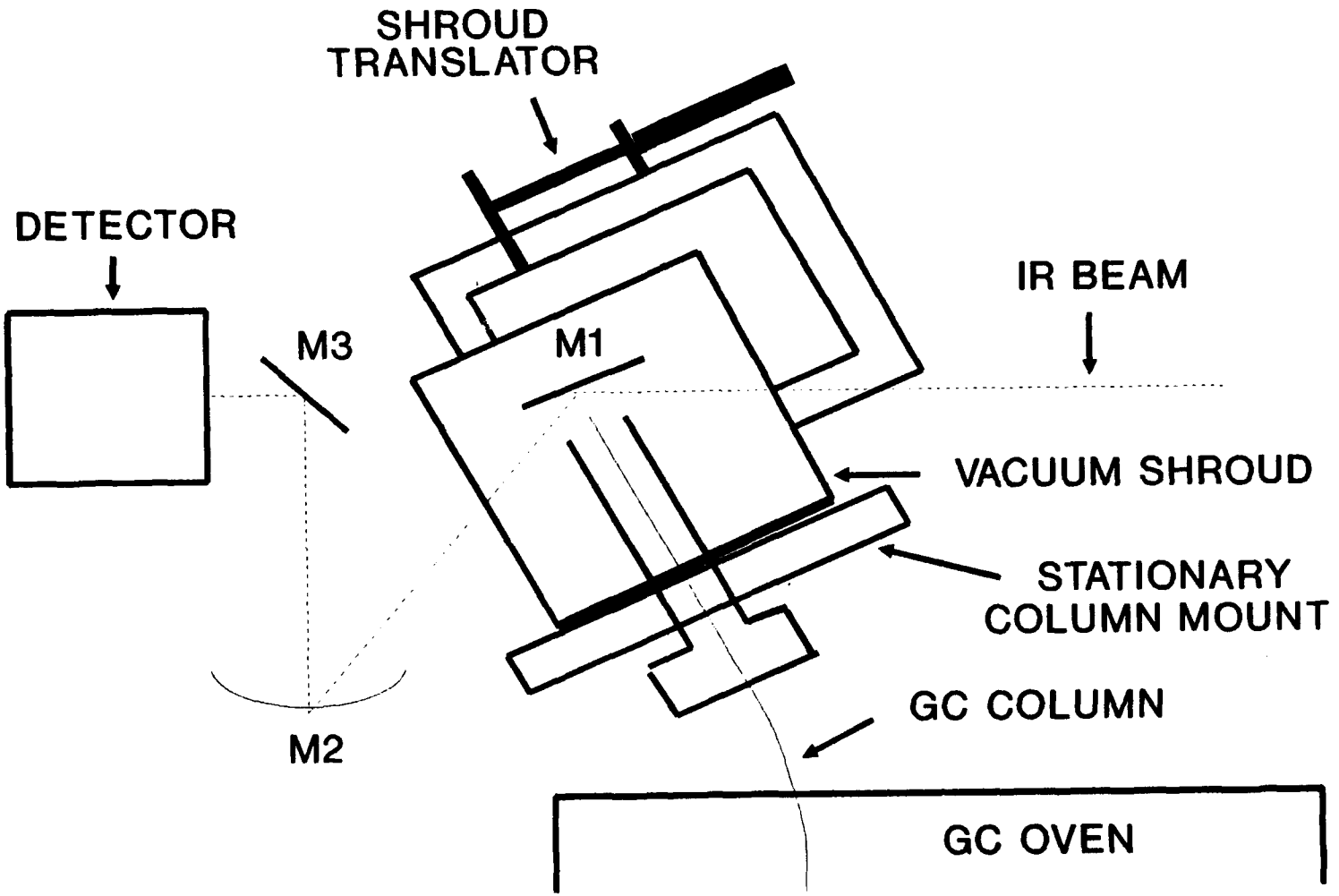

Figure 6. GC/MI/FTIR Apparatus.

to steer the infrared beam to the detector compartment of the FT-IR spectrometer and to maintain an optimum focus on the detector. Mirror M2 of Figure 6 was placed at approximately one focal length from the copper mirror to collimate the reflected infrared beam. Ideally, this mirror should be an off-axis parabola but a spherical mirror was found to be a satisfactory substitute. The collimated infrared rays were later focused onto an MCT-A detector using the focusing mirror supplied with the FT-IR instrument.

A second consequence of the FT-IR sample size limitation is that the argon carrier gas must be supplemented with a large excess of helium (which is noncondensable) to avoid producing a matrix which is too voluminous to fit between the end of the GC column and the surface of the copper mirror. It has been found (Reference 6) that a mixture of 2 percent of argon in helium is optimum under these circumstances. Alternatively, pure helium carrier gas can be used to obtain spectra of pure condensed samples (i.e. not matrix isolated). The latter option enables use of extensive commercial spectral libraries for compound identification. A library of matrix-isolation spectra is available but is too small to be of much practical use. The main advantage of matrix isolation in GC/MI/FTIR analysis lies in its ability to distinguish between molecular isomers.

A basic requirement of any GC analysis is that the output of the GC must be measured as a function of time. The simplest way to achieve this for GC/MI/FTIR is to record spectra continuously as the GC column effluent deposits onto a stationary mirror.

However, this method has two disadvangages: (1) the spectra are noisy because only a very limited amount of signal averaging can be done for any given effluent component; and (2) the sample may become totally absorbing in certain spectral regions because of accumulation of signal from many different molecular species. These problems can be alleviated by continuously moving the sample mirror as the effluent emerges from the GC column. Different species are thereby physically separated from each other on the mirror surface, and unlimited signal averaging can be done after all of the effluent has been deposited on the mirror. Figure 6 shows the apparatus that has been designed to implement this scheme. An optical translator moves the copper mirror in a plane which is parallel to the mirror surface, leaving the optical path of the infrared beam undisturbed. The GC column is held stationary during this motion by attaching it to a rigid plate that slides across an o-ring on the vacuum shroud. The optical translator can be controlled by using a computer-operated motor available commercially. The sample mirror can be accurately repositioned by the computer to any desired part of the chromatogram after the sample has been collected. Although only an x translator is shown in Figure 6, an xy translator can be substituted to make maximum use of the mirror surface.

A final requirement of the GC/MI/FTIR apparatus is that a heated interface must be inserted between the GC and MI components to accommodate the GC column. This has been done by inserting the end of the GC column through a 1/8-inch o.d. copper

tube and wrapping the tube with insulated 25-gauge nichrome wire. The nichrome leads have been connected to a variable transformer to enable heating of the interface to 200°C. The copper tube enters the shroud through a 1/8-inch Ultra-torr® stub containing a Kalrez® o-ring. The nichrome heater wire extends up to this Ultra-torr®; the final portion of the tube is short enough (about 1 inch) so that only a small drop in temperature occurs near the tip of the GC tube. Polyimide resin (Alltech Associates) provides a vacuum seal for the end of the copper tube.

SECTION III

RESULTS AND DISCUSSION

A. TANDEM FT-IR AND UV-VISIBLE EXPERIMENTS ON CONTAMINATED CLAYS

The reactivity of aromatic compounds on many types of clays results from the presence of mobile metal ions within the stacked-plate structure of the clays (Reference 7). This property has enabled clays to be used as catalysts for reactions involving aromatic organic molecules. Montmorillonite clay is particularly effective as a reaction medium because of its unusually high specific area of about 500 m^2g^{-1}. Each layer of montmorillonite consists of an aluminosilicate structure (approximate formula of $Cu_{0.25}Al_{1.5}Mg_{0.5}Si_4O_{10}(OH)_2$ for the Cu-exchanged form) in which an octahedral Mg-Al layer is sandwiched between two tetrahedral silicon layers.

An FT-IR spectrum of Cu-exchanged montmorillonite is shown in Figure 7. The most prominent feature of this spectrum is the SiO stretching vibration at 1040 cm^{-1} (Reference 8). Al-Al-OH and Al-Mg-OH bending vibrations occur at 920 cm^{-1} and 840 cm^{-1}, respectively. Hydroxyl (OH) groups in the clay lattice structure, as well as water molecules in the clay interlayers are responsible for other prominent vibrational bands. The latter produces a broad band (3600 - 2800 cm^{-1}) in the OH stretching region while the former produces a relatively sharp band at 3620 cm^{-1} . The corresponding bands in the OH bending region are not readily distinguishable.

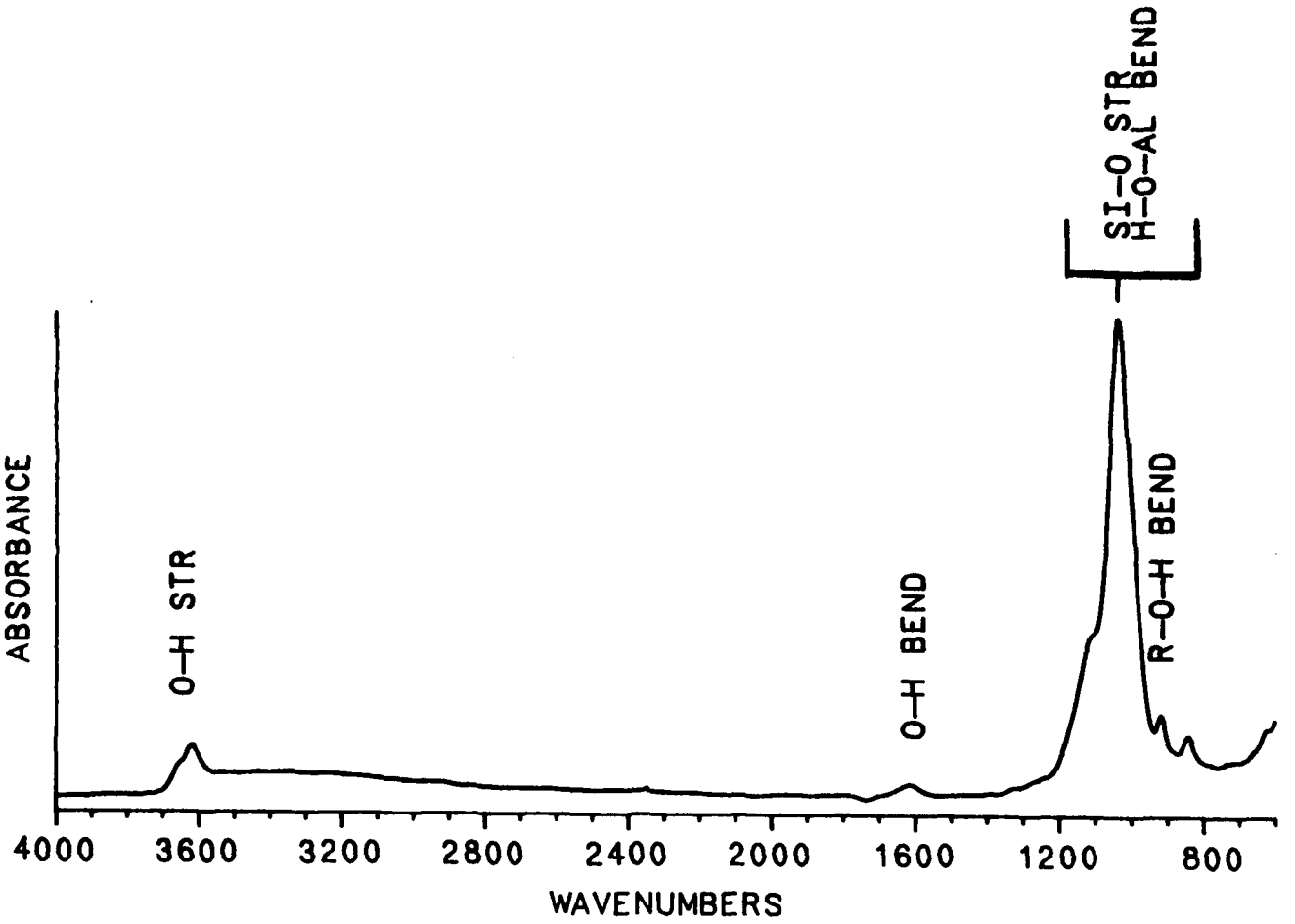

Figure 7. FT-IR Spectrum of Cu-Exchanged Montmorillonite.

The substitution of divalent Mg for trivalent Al in the octahedral layer of montmorillonite results in an excess of negative charge in the interlayers. This charge imbalance induces other positively charged atoms to intercalate into the interlayers of the clay, resulting in a highly acidic substrate. Ions commonly found in the interlayers of natural clays include Na^{+}, Ca^{++}, Cu^{++}, and Fe^{+++}. Under typical natural conditions, these ions are surrounded by water molecules and the clay is inert to most aromatic molecules. However, under warm and/or dry conditions, many aromatic molecules have been found to undergo a charge transfer with transition metal ions such as Cu^{++} and Fe^{+++}. A schematic diagram of this charge transfer is shown in Figure 8 for benzene in Cu-montmorillonite.

The first system selected for the tandem FT-IR/UV-VIS experiments was p-dimethoxybenzene (DMOB) on Cu-montmorillonite (CUM). A brief discussion of this system is given below. A more thorough discussion has been presented elsewhere (Reference 9).

Figure 9 shows the growth of infrared bands on CUM as a function of the time of exposure to DMOB in the presence of P_2O_5 desiccant. For this experiment, the clay film was supported on a polyethylene substrate since it was too thin to be self-supporting. A remnant of a subtracted polyethylene absorption band can be seen at 1470 cm^{-1}. Vapor-phase DMOB did not have to be subtracted since it was too weak to be observable. The disproportionate growth of the bands in this spectrum indicates that at least two species are present. One of these species can be identified as physisorbed

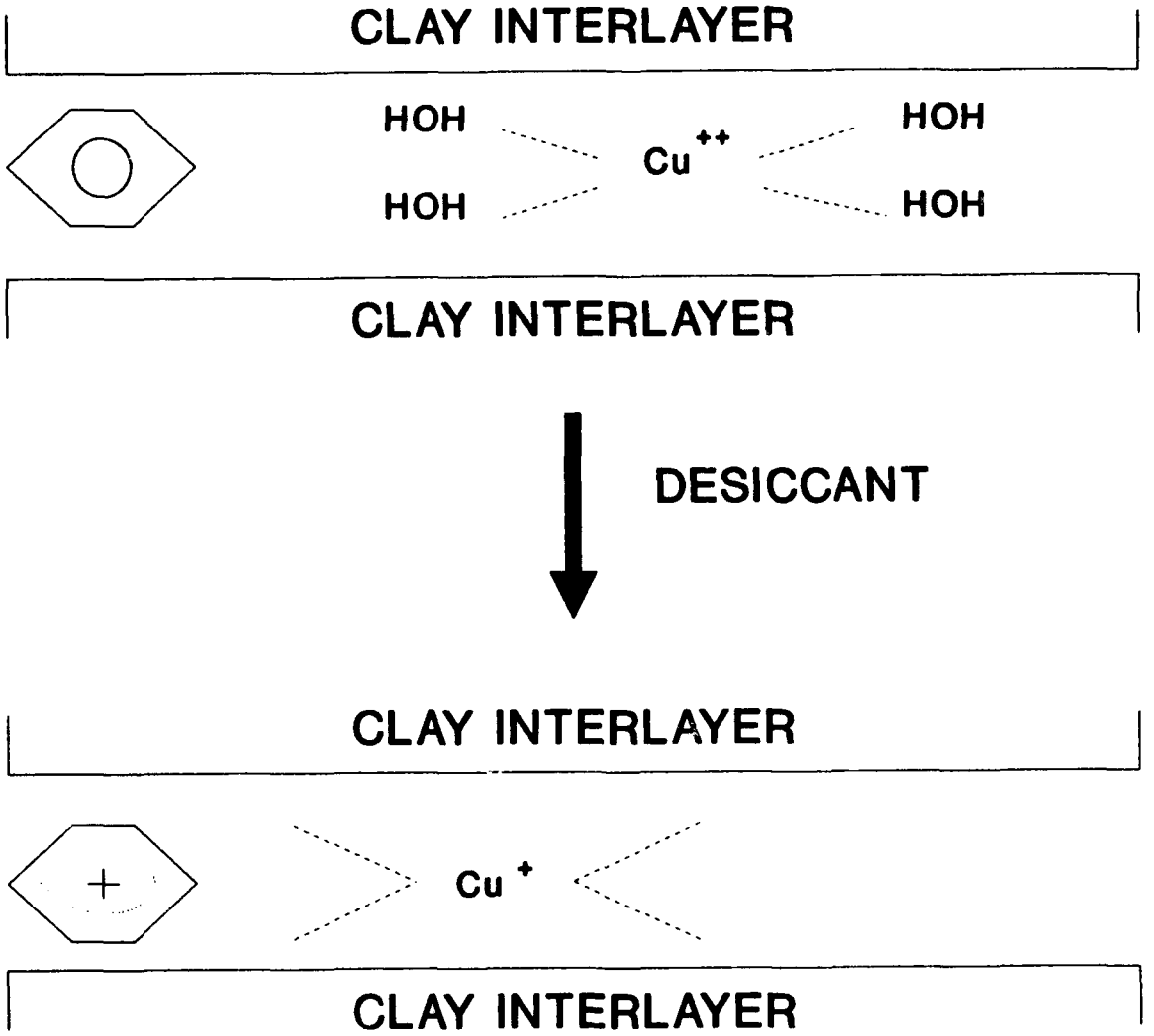

Figure 8. Charge-Transfer Reaction for Benzene on Cu-Montmorillonite.

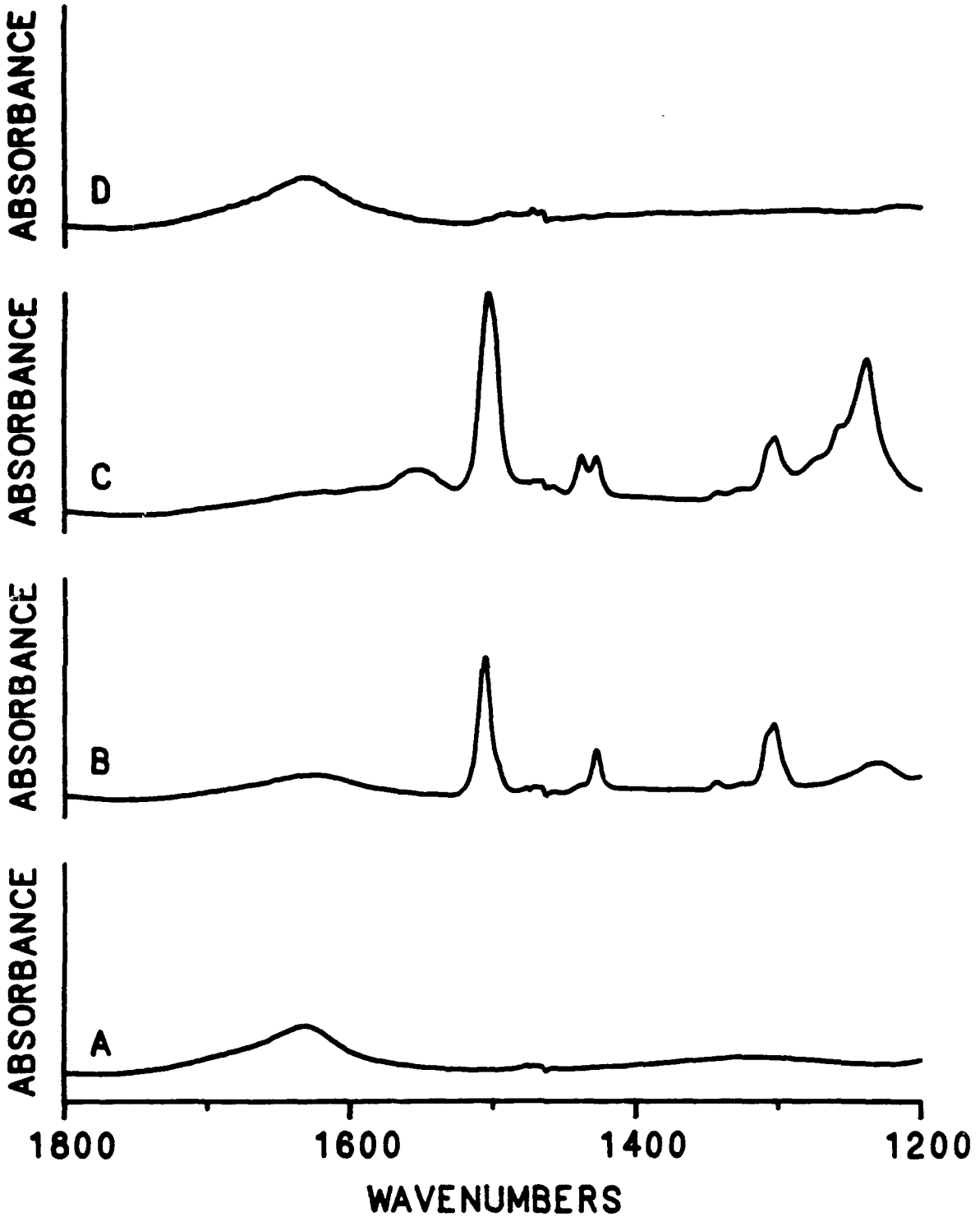

Figure 9. FT-IR Spectra of Cu-Montmorillonite + DMOB + P_2O_5: A) at 0.0 Hr with Only Clay Present, B) at 3.0 Hr, C) at 69 Hr, D) After Reintroduction of Ambient Air and Removal of DMOB.

DMOB by comparison with a reference spectrum of a pure solid DMOB sample. Another can be identified as the cation of DMOB by comparing the UV-VIS spectrum of the clay sample with that of the spectrum of the DMOB cation that has been published in the manual of Shida (Reference 10).

A comparison of UV-VIS data of DMOB with corresponding FT-IR data is given in Figure 10. Part of the infrared spectrum was deleted from this figure because it contained strong absorption from the polyethylene substrate. The growth of the infrared bands in the 1525 cm^{-1} to 1200 cm^{-1} region is in qualitative agreement with the growth of the DMOB cation bands at 440 nm and 460 nm. Unfortunately, the UV-VIS bands were too strongly absorbing to permit a more accurate comparison.

The DMOB/CUM system is particularly simple because no reaction takes place other than a transfer of charge from the Cu++ ions on the clay to the aromatic molecules. Examinations of more complicated systems such as benzene/CUM and toluene/CUM are planned.

The spectroscopic absorption of an aromatic compound on a clay can be obtained as a function of adsorbed mass by interfacing a clay-film cell to a microbalance. Such an apparatus is in use at the University of Florida and is described in the literature (Reference 9). A similar cell is planned for use at Tyndall AFB.

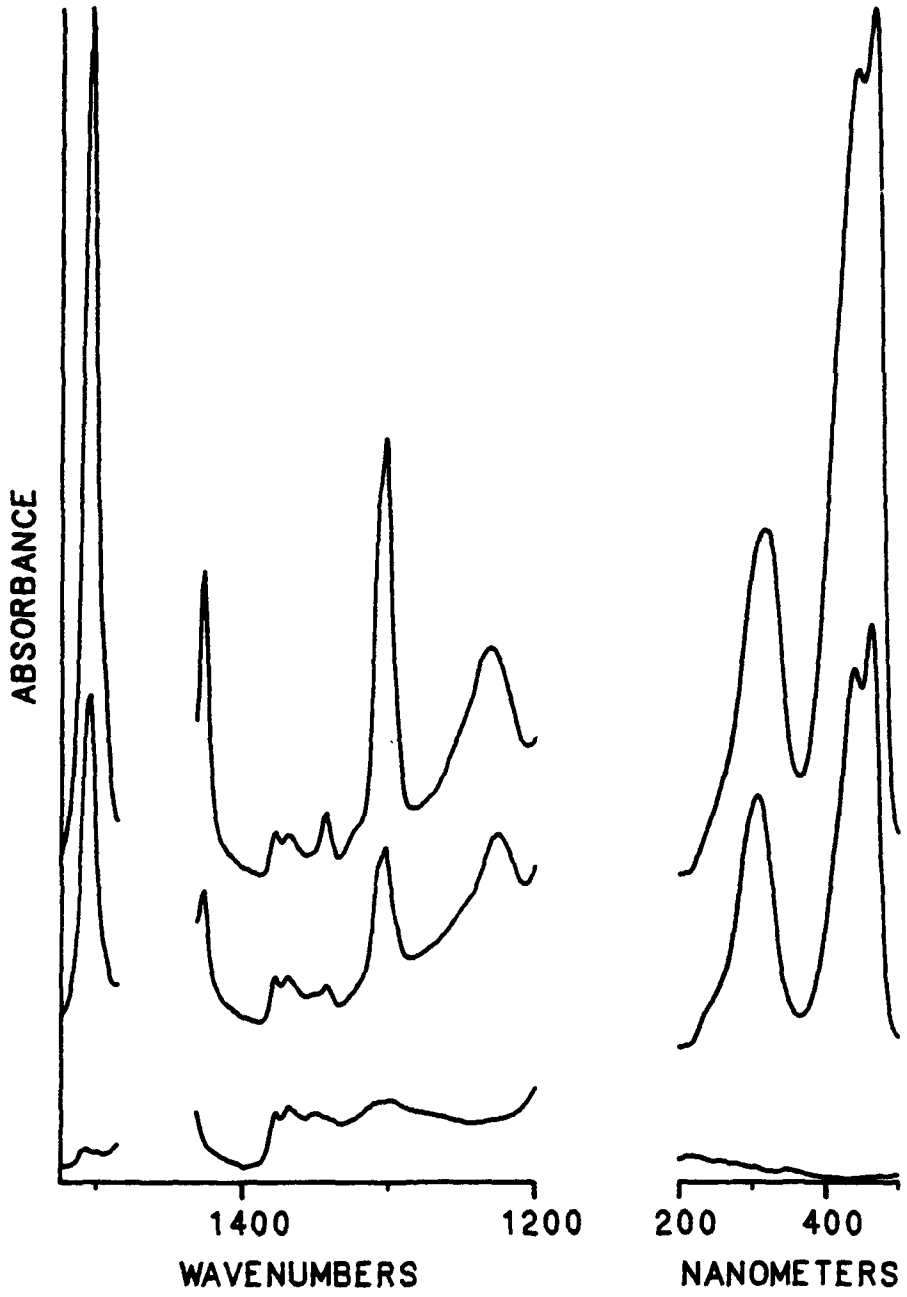

Figure 10. Growth of FT-IR and UV-VIS Bands of a DMOB/CUM Film as a Function of Elapsed Time of Dehydration: A) 0.1 Hr, B) 2.0 Hr, and C) 3.0 Hr.

B. ANALYSIS OF CLAY EXTRACTS

Examples of data collected during a typical clay extraction are shown in Figures 11 and 12. Figure 11 compares the FT-IR spectrum of a toluene-contaminated CUM sample with the corresponding spectrum of the acetone extract of this sample. The infrared absorption of the contaminant mixture is much stronger in the extract than in the original sample because the contaminant is much more concentrated in the former case. The relative intensities of absorption bands in the two spectra are not the same because the acetone extracted the components of the contaminant mixture with varying degrees of efficiency.

A GC/MS analysis of the extract yielded the chromatogram shown in Figure 12. This chromatogram has not yet been fully analyzed but the strongest peak has been identified as 1-methyl-2-phenylmethylbenzene, which is a toluene dimer. This result is in accordance with previous reports of multimer formation for some aromatic compounds adsorbed on CUM (References 11 and 12).

C. MATRIX-ISOLATION EXPERIMENTS WITH HEATED SAMPLES

The sample heater described in Section II-D was ineffective in separating the components of clay extracts because the differences between the vapor pressures of the components was not sufficiently diverse. However, the heater appears to be useful

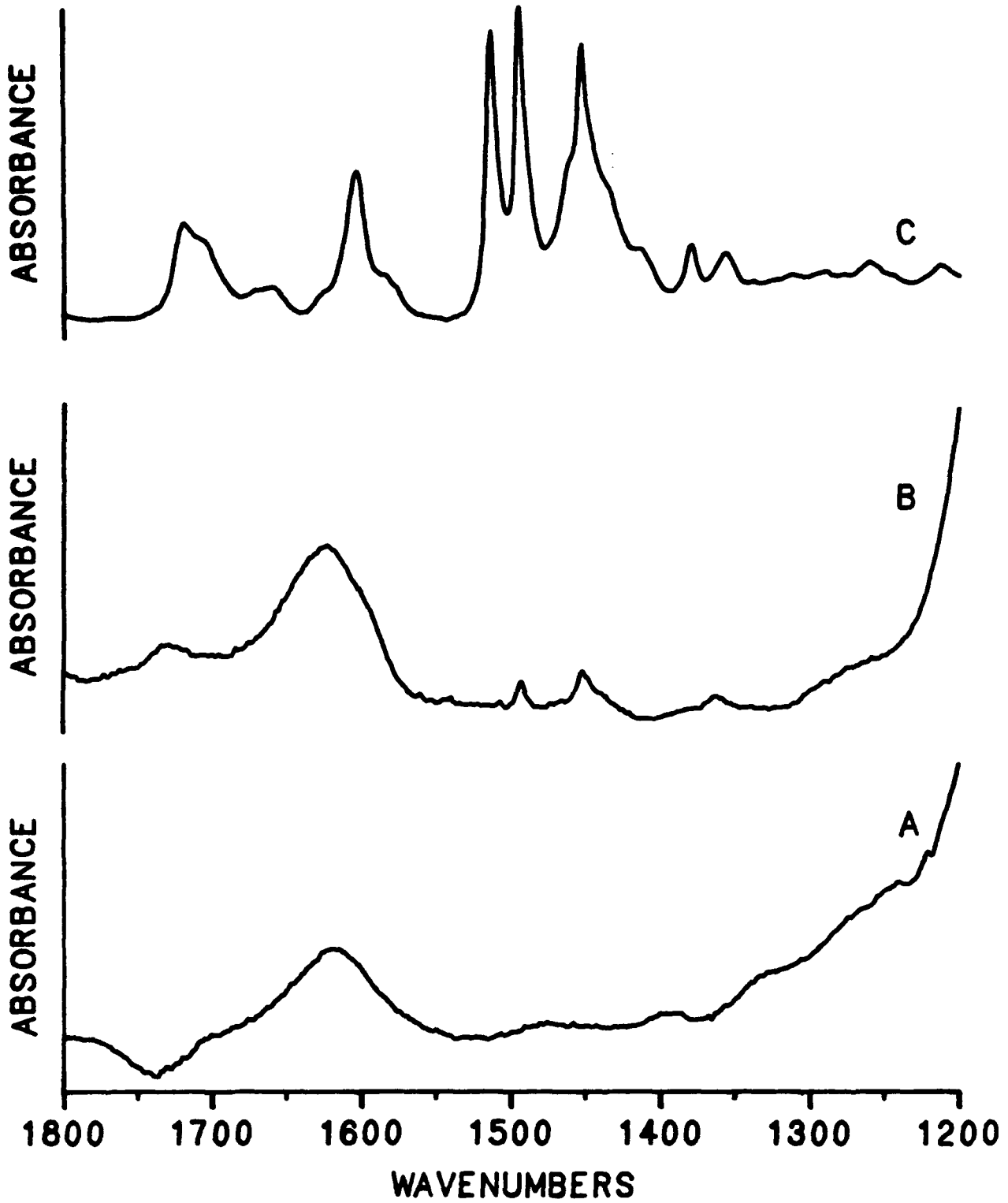

Figure 11. FT-IR Spectra of: A) Cu-montmorillonite in Ambient Air, B) Cu-montmorillonite After Refluxing in Toluene, and C) An Acetone Extract of Toluene-Contaminated Cu-Montmorillonite.

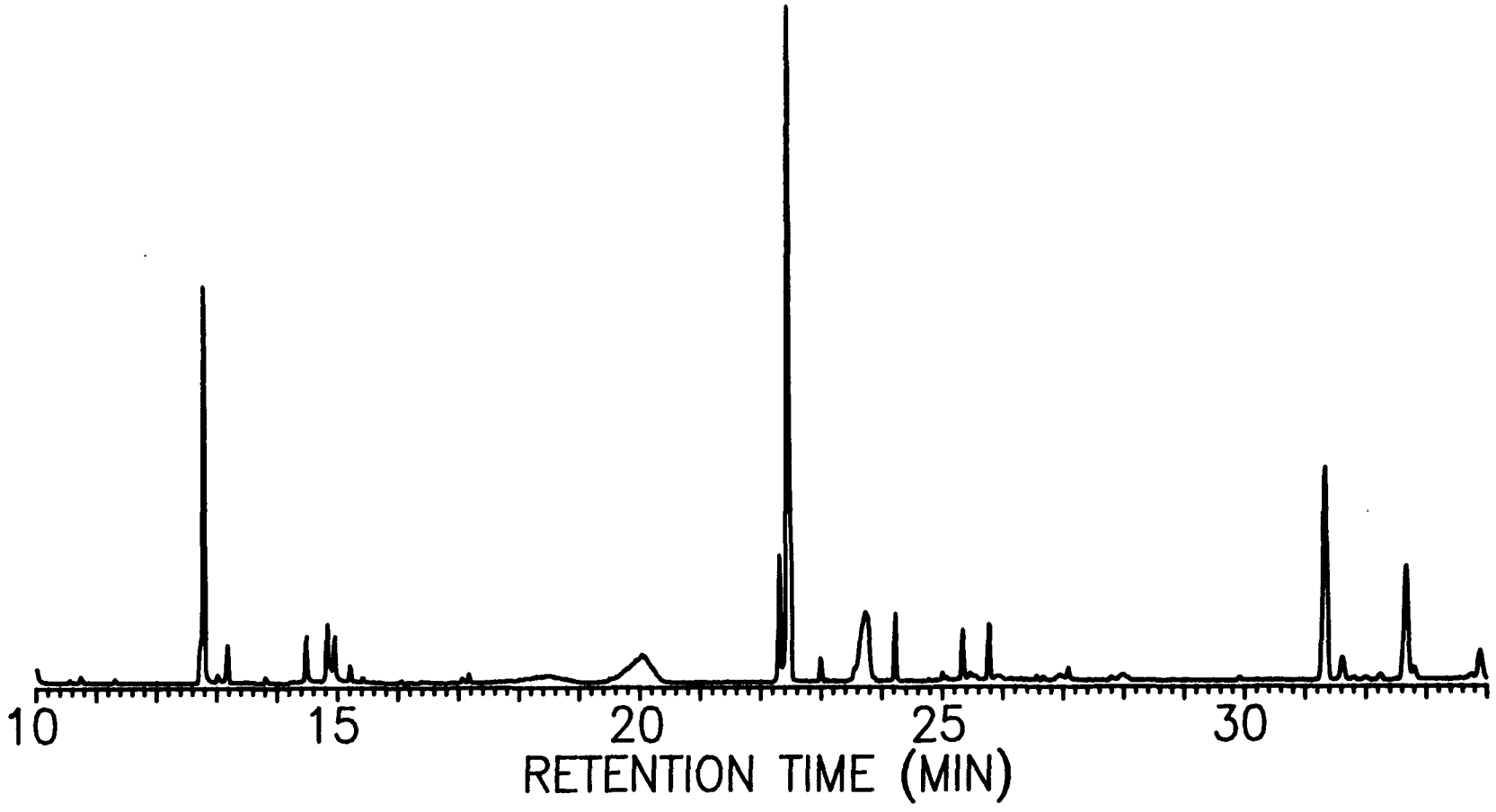

Figure 12. GC/MS Chromatogram for Acetone Extract of Toluene/CUM.

for obtaining reference spectra of pure compounds of low volatility.

SECTION IV

CONCLUSIONS

Two accomplishments have been made toward understanding the behavior of aromatic compounds on soils at the molecular level:

1. The analysis of a simple system: DMOB/CUM. For this system, reaction occurs only under very dry conditions, and proceeds only to the point where a charge transfer takes place between the Cu^{++} ions and the DMOB to form Cu^{+} and $DMOB^{+}$. As soon as water is reintroduced, the $DMOB^{+}$ cations revert back to neutral DMOB. This behavior seems to be characteristic of para-substituted be e compounds (References 3, 9, 13, and 14).

2. The implementation of methods for extracting reaction products from clays and analyzing the extracts. The analysis of complex reactions on clays would be prohibitively difficult without the capability of separating components of reaction-product mixtures. Soxhlet extractions have been applied with some success and may soon be supplemented with SFE. GC/MS has proven effective in identifying some components of clay extracts and will shortly be complemented with the GC/MI/FTIR technique. These methods will be useful in analyzing systems such as toluene/CUM and benzene/CUM, where formation of multimers (i.e. dimers, trimers, ...polymers) has been reported (References 2, 11, and 12).

SECTION V

FUTURE PLANS

One near-term objective is to combine the SFE and GC/MI/FTIR techniques with traditional methods to analyze clay/aromatic systems in which a multitude of reaction products is formed. A second is to combine gravimetric measurements with FT-IR spectroscopy to relate a bulk property of a clay (grams of contaminant sorbed) to a molecular-level property (spectroscopic absorption).

Once an understanding of a few representative clay/aromatic systems has been achieved, it should be possible to predict the behavior of similar systems. The complexity of the systems will then be increased by replacing the clays with natural soil samples, and by using multicomponent fuels instead of individual aromatic compounds. A contaminant-transport model generated from these studies should be superior to empirical models based on bulk measurements since the latter may be based on false assumptions of molecular-level interactions and cannot be extrapolated with confidence.

One possible by-product of studies on contaminated clays might be the development of an artificially modified clay that efficiently traps any aromatic fuel molecules that sorb onto it. Such a clay could be used to contain a fuel spill within a localized area. One way of producing such a clay is to introduce

surfactants. Much research is already underway in this area (e.g. see Reference 15).

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APPENDIX A

PROGRAM DESCRIPTIONS AND SOFTWARE CODES FOR THE WORK STATION OF THE NICOLET MODEL 740 FT-IR SPECTROMETER

Appendix A contains:

1. An alphabetic listing of user-defined macrocommands executed from the FT-IR SX operating system.
2. A list of FORTRAN programs and commands that are executed from the NICOS operating system.
3. An alphabetic listing of macro software codes.
4. An alphabetic listing of FORTRAN software codes.

Each macro command given below is followed by :

1. A list of submacros, if any.
2. A list of FORTRAN programs and NICOS data files used by the macro.
3. A brief description of the macro.

The names of all of the listed macros obey the following rules:

1. They consist of three alphanumeric characters.
2. They identify the macro as a parent macro or a submacro depending on whether the third character is a letter or number, respectively.
3. Wherever possible, they alphabetically group the parent macros with their associated submacros. Exceptions occur when a submacro belongs to more than one parent macro, and when the submacro is a conditional macro.

ABL Blanks absorbance file DFN. It is used for clearing out a file prior to sending FORTRAN output to it.

AOB SB1, SBFTYP.FCP
Converts a single-beam file (RFN) to "auto-absorbance" (DFN) using the maximum intensity between XSP and XEP as the background for RFN.

ALN M17, M19, SA0; TMXFTR.GCP
Aligns the "fixed" mirror of the interferometer. It is essentially the same as the system macro of the same name except that it allows the detector, resolution, and aperture to be changed without running a separate macro.

ASC Compresses a block of scratch files into an ASCII file and directs the output through the printer port to a logging

file on a second computer. If no output is obtained, toggle the DCE/DTE switch next to the printer port. If strange characters are produced, set the receiving computer to "parity = none". If some of the data gets lost, reduce the baud rate of the Nicolet computer. The program can be tested by sending the output to a Nicolet printer instead of a second computer.

ATG AT1, AT2. AUTIT.FCP, AUTIT1.FCP
This is a documentation macro only. It describes how to generate automated titles in the course of executing an automated data-collection macro such as SAM. When this procedure is implemented, file titles can be generated which include automatically incremented file extensions, collection dates, and elapsed times. Since the file title is restricted to 40 characters, it may not always be possible to select all of the possible options that are available.

BAK SA0, M17, M23
Collects and displays a background spectrum. The interferogram is copied to Nicos file I.EXT[,IRDATA] so that the raw data can later be saved on floppy disk, if desired. The single-beam spectrum is placed in file BFN.

BCR BC1
Corrects a spectrum baseline interactively. It divides the spectrum into several segments and prompts the user to correct these segments individually.

BLX BLANKX.FCP, FTPARM.FCP
Blanks several wavenumber ranges of a spectrum. It is useful for plotting a spectrum in which the absorbance is off scale in some wavenumber ranges.

BLZ BLANKZ.FCP, BLANK.DAT
Sets the absorbance to zero over selected wavenumber ranges of an absorbance file, and uses baseline adjustment to avoid sudden offsets in the y-axis at the ends of the wavenumber ranges. It is useful for extracting the spectrum of one compound from those of other compounds present in the same sample.

BSL ABL, BS0-BS2, M20-M21; BASLIN.DAT, BASLIN.FCP, FTPARM.FCP, MATINV.FCP, SPLINE.FCP
Corrects the baseline of an absorbance spectrum automatically. It is intended for eliminating fringes from matrix-isolation spectra. It resets the absorbance to zero at the minimum absorbance point in every equally sized block of words in a spectrum; and applies cubic spline interpolation to generate a baseline for all other points. The baseline points are sent to BASLIN.DAT and to scratch file 0 so that badly chosen points (e.g. those that are within a molecular absorption band) can be deleted and the

baseline recomputed. Subtraction of water and carbon dioxide absorption should be performed (using SVI or SVP) prior to running this program. This program is unsuitable for spectra having many wide absorption bands.

DCP Scales several absorbance spectra so that a specified reference peak appears to have the same absorbance on the display screen for all of the spectra. The scaling affects only the screen display, and does not alter any stored files.

DER RESOLU.FTN
Deresolves an absorbance file to 16 wavenumbers resolution for library searches, using software supplied by Nicolet.

DSC DS1
Compares successive fragments of two files (RFN and DFN) on the display screen using constant absorbance per inch. The minimum absorbance is obtained separately for RFN and DFN by autoscaling. The maximum absorbance is obtained for RFN by autoscaling, and for DFN by adding the range of RFN to the minimum absorbance of DFN. This scheme enables comparison of spectra having markedly different baselines.

DUM This is a dummy macro used to document all other macros.

EMP M99; EMPFIL.FCP
Copies a spectral file into all vacant files in a block of scratch files. This prevents an "invalid fsb" message from occurring during execution of the TTL macro.

FSP FSPRN.FCP
Lists a sector of scratch file data on the display screen.

ITG INTGRL.FCP, INTSEG.DAT
Integrates selected wavenumber ranges of an absorbance file and sends the output to the printer. These ranges must first be entered into Nicos file "INTSEG.DAT" using the formatting described in INTGRL.FOR.

LBI LB1, LB2
Moves a block of I.EXT[,IRDATA] interferogram files created by macros "BAK", "STI", or "SAM" to a user-specified location after initially transferring them to a block of scratch files. It is important to select the intermediate scratch files so that no important spectra are overwritten.

LBM LB1, LB2
Copies a block of scratch files to a user-specified disk location.

LTR LETTERS.FCP, GPLOT.LIB[HLIB,ZETA8]
Sends text from the keyboard to the plotter. The size and orientation of the letters are user-specified. This macro

is needed for adding text to rotated plots created by macros PLI and PLC since these plots are oriented differently that the rotated plots produced by Nicolet's software.

NSF Copies a block of files from Nicos to the scratch area.

NXP Advances the page of the Zeta-8 plotter.

PCP PC1
Performs the same function as macro DCP except that the output for PCP goes to the plotter.

PFB BENPAR.740
Reads parameter file PFN of BENPAR.740, and prints pre-selected parameters.

PLC PL1-PL4, PL7, M30-M32, M40-M49; AXIS2.FCP, FSBTIT.FCP, GPLOT.LIB[HLIB,ZETA8], PLOTFT.FCP, PLT.DAT, PLPARR.FCP, PLPARW.FCP
Compares several plots on one x-axis. It enables the user to control plot parameters to the fullest extent permitted by standard FORTRAN plotting subroutines. Many of the standard FTIR parameters are redefined within this program; the initial settings of these parameters are therefore saved at the beginning of this program in PFN=49, and retrieved after the plotting is over. All of the plotting parameters are read from macros rather than from FORTRAN subroutines so that the user can reorganize the setup of the program without editing FORTRAN programs. For example, the user can easily change a defaulted parameter by inserting an extra line of keyboard input. Plotting parameters are saved in NICOS file PLT.DAT each time PLC is executed so that the program can be rerun with these parameters without having to reenter them.

PLI PL1-PL6, M40-M46, M48-M49; AXIS2.FCP, FSBTIT.FCP, GPLOT.LIB[HLIB,ZETA8], PLOTFT.FCP, PLT.DAT, PLPARR.FCP, PLPARW.FCP.
Plots N files on N x-axes. Otherwise, PLI uses the same algorithms as PLC.

PMY Prints y-axis limits for a block of FTIR files using multiple screen displays.

PPP PP1
Plots an FTIR file and prints wavenumbers of spectral peaks.

RES RESOLU.FTN
Changes the resolution of an absorbance file using software supplied by Nicolet.

R#W PFB

Sets the resolution by reading a parameter file. The "#" character of R#W is a code that designates a parameter file, and consequently, the resolution. The codes are set at 0, 1, 2, 3, or 4 for resolutions of 0.5, 1, 2, 0.3, and 4 wavenumbers, respectively. The R#W macros can be used in conjunction with the ASG command to enable the resolution to be set by pressing a single key.

SAM SA0, SA2-SA5, SA9, M12-M15, M17, M50-M52; AUTIT.FCP, AUTIT1.FCP
Collects, displays, and auto-titles a block of sample spectra. Delay times between spectra can be chosen to be automated or manual. Input can be read from a file of default parameters (M51 or M52) if desired. Two screen displays of the spectrum are presented so that both a full spectrum and a magnified segment of the spectrum can be obtained without using cursor keys.

SBS SB0-SB1; SBFTYP.FCP
Regenerates a single-beam file from an absorbance file (DFN) and a second single-beam file.

SMH SMOOTH.FTN
Smoothes a spectrum using Nicolet's software.

STI SA0, SA2-SA5, SA9, M12-M15, M17, M23, M50-M52
Collects, displays, and manually titles a block of sample spectra. Except for titling, STI is identical to SAM.

STK STICK.DAT, STICK.FCP
Generates a stick spectrum from absorbance data in Nicos ASCII file STICK.DAT. See directions in STICK.FOR for setup of STICK.DAT.

SUM SU0; SUMSPC.FCP
Similar to Nicolet's ADD operation except that the output goes to a new scratch file, and a constant value can be added to a spectrum.

SVI SV0-SV3
Interactively subtracts individual water and carbon dioxide vapor bands from an absorbance spectrum using reference spectra from the [ROOT,VAPOR] subdirectory. The generic names of the reference spectra are listed within the SVI program. The file extensions are set to either 0 or 2 for resolutions of 0.5 and 2 wavenumbers, respectively, using a formula listed in submacro SV3. For other resolutions, it is necessary to create additional reference spectra (e.g. by using the RES macro) whose names are compatible with the SVI macro.

SVP SV0-SV3

Interactively subtracts water and carbon dioxide vapor bands using one multiplier for each of these two molecules. Otherwise, SVP is identical to SVI.

TTL Prints a block of FTIR file titles and starting times using multiple screen displays.

FORTRAN PROGRAMS RUN FROM NICOS

AMAC.FOR This program alphabetizes a macro directory by alphabetizing the ASCII file MACROSAVE created from MACTBL and MACDIR. MACROSAVE must first be generated via the following set of NICOS commands:

```
COPY MACTBL/MACTBL.SAV
COPY MACDIR/MACDIR.SAV
MACGET
@MACROSAVE
```

The macros comprising MACROSAVE are sent to a set of generic files called JUNK, and then transferred alphabetically to output file AMAC.NEW. After the program has ended, the intermediate JUNK files can be deleted by using the command:

```
DEL JUNK.*:D
```

To complete the replacement of the old macro directory with the alphabetized directory, it is necessary to apply the KIL command to the old macro directory and then read the AMAC.NEW file with the MACCRT command.

BAUD# (where # = 300, 600, 1200, 2400, 4800, 9600) These programs reset the baud rate of the printer port. They are needed whenever there is a mismatch between the default baud rate of the printer port and whatever device is attached to the printer port. Each of these programs consists of just two steps:

```
363 WDVS
# WDEV
```

where # is a code for the baud rate. These codes are defined as follows:

#	BAUD RATE
6	300
7	600

10	1200
12	2400
14	4800
16	9600

PMAC.FOR This program prints a NICOS file containing multiple macros using format specifications entered from the keyboard.

```
!ABL
DUM. "ABL" < BSL
DUM. BLANKS ABSORBANCE FILE DFN.
TXD
FCD=-1
MUD
ABD
END


!ALN
DUM. "ALN" > SA0, M19
OMD
***  FTIR 740 ALIGNMENT MACRO  ***
OMD
*
PFN=49
SPF
CSN=2
SA0
OMD
DETECTOR:
DET
OMD
APERTURE (SM, MD, OR FL):
APT
OMD
DOES THE SELECTED APERTURE DIFFER FROM THE CURRENT
OMD
PHYSICAL STATE OF THE IRIS (0=NO, 1=YS)?
CMP=0
CMP
CMP=CMP*19
DUM: CMP=0 (DUMMY) OR 19 (COLLECT 1 SCAN)
CMR
VI0=0
VI1=3
VI2=5
VI3=NDP
GFN
TMXFTR.GCP
FRN
NDP=VI3
PFN=49
SPF
END


!AOB
DUM: "AOB" > SB1
OMD
```

```
MACRO CONVERTS 1-BEAM FILE (RFN) TO "ABSORBANCE" (DFN) USING
OMD
THE MAX INTENSITY BETWEEN XSP & XEP AS THE "BACKGROUND" FOR RFN.
OMD
*
OMD
1-BEAM INPUT FILE:
RFN
OMD
ABSORBANCE OUTPUT FILE:
DFN
OMD
CM-1 RANGE OF INTEREST:
XSP
XEP
SB1
ASD
DSD
END



!ASC
OMD
"ASC" COMPRESSES A BLOCK OF SCRATCH FILES INTO AN ASCII FILE
OMD
& DIRECTS THE OUTPUT THROUGH THE PRINTER PORT TO A 2ND COMPUTER.
OMD
(1) CONNECT THE PRINTER PORTS OF THE 2 COMPUTERS
OMD
(2) SET THE NICOLET PRINTER PORT SWITCH TO "DCE"
OMD
(3) SET UP A LOG FILE ON THE HOST COMPUTER WITH "PARITY = NONE"
OMD
# OF FILES (MAX=7):
QIT
OMD
1ST FILE:
DFN
PAD
OMD
1ST (FXF) & LAST (LXF) CM-1:
FXF
LXF
OMD
PRESS <CR> TO BEGIN EXECUTION
PAU
GFN
ASCSND.FCP
FRN
END
```

```
!ATG
DUM: "ATG" > AT1,AT2
OMD
*
OMD
*** AUTOMATIC TITLE GENERATION FOR FTIR FILES ***
OMD
*
OMD
THIS IS A DOCUMENTATION MACRO ONLY.  GENERATING TITLES REQUIRES
OMD
INSERTION OF AN IMD COMMAND AND A FRN COMMAND (FOR ATG.FCP) AT
OMD
SEPARATE LOCATIONS IN A PROGRAM THAT COLLECTS A BLOCK OF
OMD
SPECTRAL FILES.  SRT & DFN MUST BE SET TO THE INITIAL & CURRENT
OMD
FILES OF THIS BLOCK.
OMD
THE MACRO DESRIPTOR OF DFN IS USED TO STORE THE KEYBOARD INPUT
OMD
SPECIFICATIONS FOR THE TITLES OF THE SPECTRAL FILES.
OMD
*
OMD
GIVE 5 DATA FIELDS OF TITLE INFORMATION, USING ASTERISKS TO
OMD
SEPARATE THE FIELDS.  USE CONSECUTIVE ASTERISKS TO SPECIFY AN
OMD
EMPTY FIELD.  TYPING JUST [CR] IS ACCEPTABLE, AS IS OMITTING
OMD
EVERYTHING AFTER THE GENERIC FILE DESCRIPTOR.
AT1
END



!AT1
DUM: "AT1" < ATG
OMD
*
OMD
FIELD #1:  GENERIC FILE NAME
OMD
FIELD #2:  INITIAL FILE EXTENSION #
OMD
FIELD #3:  GENERIC FILE DESCRIPTOR
OMD
FIELD #4:  REFERENCE TIME FROM WHICH TO COMPUTE AN ELAPSED TIME;
OMD
           SPECIFY WITH AN 8-INTEGER # IN ACCORDANCE WITH THE
OMD
```

```
            FOLLOWING EXAMPLE:
OMD
*
OMD
            MAY 6 11:03  BECOMES  05061103
OMD
*
OMD
FIELD #5:  "D" FOR DATE
AT2
END



!AT2
DUM: "AT2" < ATG
OMD
*
OMD
             EXAMPLE OF FULL TITLE SPECIFICATION:
OMD
*
OMD
                    HZ*1*AIR OXID*05061103*D
OMD
*
OMD
NOTE THAT THE TITLE IS RESTRICTED TO 40 CHARACTERS.
END



!BAK
DUM: "BAK" > SA0,M17,M23
OMD
*** "BAK" COLLECTS & DISPLAYS BACKGROUND SPECTRA ***
OMD
*
OMD
CHOOSE RESOLUTION CODE:
OMD
   CSN   CM-1
OMD
    0    0.5
OMD
    1    1
OMD
    2    2
OMD
    3    0.3
OMD
    4    4
CSN
```

```
SA0
OMD
DETECTOR:
DET
TEM=100
NPR
OMD
FILE #:
BFN
OMD
APERTURE (SM, MD, OR FL):
APT
DUM: AFP OPERATES ON DFN.
VI0=DFN
DFN=BFN
OMD
# OF SCANS:
NSB
OMD
CM-1 LIMITS FOR SCREEN DISPLAY:
XSP
XEP
CLB
CMP=23
CMR
GFN
I.001[,IRDATA]
EXT=BFN
AFP
OMD
INTERFEROGRAM SENT TO [,IRDATA]
FPB
ASB
DSB
DFN=VI0
END


!BCR
DUM. "BCR" > BC1.
OMD
**** INTERACTIVE BASELINE CORRECTION ***
OMD
FILE #
DFN
OMD
1ST % LAST CM-1 OF THE FULL SPECTRUM:
FXF
LXF
BC1
OMD
USE X/Y ROLLS, X/Y ZOOMS, & CONTROL U TO DETERMINE CM-1 RANGES
```

```
OMD
TO BE CORRECTED. RECORD THE CM-1 FOR LATER USE. THEN HIT [CR].
PAU
OMD
# OF CM-1 RANGES TO BE CORRECTED:
QIT
FOR AAA=1 TIL QIT
OMD
INITIAL & FINAL CM-1 OF A SEGMENT TO BE CORRECTED:
XSP
XEP
OMD
USE X-ROLL, Y-ROLL, & Y-ZOOM ON BASELINE.  SAVE WITH CONTROL Z
BLC
VF0=XSP
XSP=XEP
XEP=VF0
NXT AAA
BC1
END


!BC1
DUM. "BC1" < BCR
XSP=FXF
XEP=LXF
ASD
DSD
TEM=100
NPR
END


!BLX
DUM. "BLX"
OMD
*** SPECTRUM BLANKING MACRO ***
FXF=XSP
LXF=XEP
TEM=100
NPR
OMD
FILE TO UNDERGO PARTIAL BLANKING:
DFN
PAD
OMD
# OF CM-1 RANGES TO BE BLANKED:
QIT
GFN
BLANKX.FCP
FOR III=1 TIL QIT
```

```
OMD
ENTER A PAIR OF BLANKING RANGE LIMITS (CM-1):
XSP
XEP
FRN
NXT III
XSP=FXF
XEP=LXF
ASD
DSD
END


!BLZ
OMD
"BLZ" BLANKS SELECTED PORTIONS OF AN ABSORBANCE FILE BY SETTING
OMD
ABS=0 & USES BASELINE ADJUSTMENT TO AVOID SUDDEN OFFSETS IN THE
OMD
Y-AXIS AT CM-1 RANGE LIMITS.  SEE DOCUMENTATION IN "BLANKZ.FOR"
OMD
FOR SETUP OF THE "BLANK.DAT" NICOS INPUT DATA FILE.
OMD
INPUT (SFN) & OUTPUT (DFN) FILES:
SFN
DFN
OMD
DATA SET # OF "BLANK.DAT" FILE:
VI2
MSD
PAD
TXD
GFN
BLANKZ.FCP
FRN
ABD
END


!BSL
DUM. "BSL" > BS0-BS2,ABL,M20-21
OMD
AUTOMATED BASELINE-CORRECTION PROGRAM "BSL".
BS0
DUM. 'MRD' ENSURES VALID FSB'S:
MRD
MNT=DFN
DFN=OFN
MRD
ABL. BLANK FILE OFN
DFN=MNT
GFN
```

```
BASLIN.FCP
FRN
BS1
BS2
END


!BS0
DUM. "BS0" < BSL
OMD
USE EXISTING "BASLIN.DAT" (VI1=0) OR CREATE FILE (VI1=1)?
VI1
CMP=VI1*21
CMR
OMD
ABSORBANCE INPUT FILE:
RFN=5
PRN RFN
OMD
OUTP      OR ABSORBANCE (DFN) & BASELINE PT DISPLAY (OFN):
DFN=c
PRN D.
OFN=0
PRN OFN
PAR
OMD
1ST & LAST CM-1:
FXF=XSP+1
LXF=XEP-1
PRN FXF
PRN LXF
OMD
RESET INPUT (0 OR 1)?
CMP=0
CMP
CMP=20*CMP
CMR
END


!BS1
DUM. "BS1" < BSL
DUM. COMPARES SUCCESSIVE FRAGMENTS OF DFN & RFN USING CONSTANT
DUM. ABS/INCH (CF. "DSC"), ALONG WITH FILE OFN WHICH CONTAINS
DUM. BASELINE REF PTS GENERATED BY "BASLIN.FOR".  THE DISPLAY
DUM. BEGINS AT XSP.
VI1=SFN
VI2=XSP
VI3=XEP
OMD
****
```

```
SFN=OFN
OMD
CM-1 RANGE PER SCREEN DISPLAY (- SIGN FOR DECREASING CM-1):
VF1=-400
VF1
XEP=XSP+VF1
OMD
# OF DISPLAY RANGES:
QIT=9
QIT
TEM=9
FOR III=1 TIL QIT
BS2
NXT III
SFN=VI1
XSP=XSP-VF1
XEP=XEP-VF1
END


!BS2
DUM. "BS2" <BSL
ASR
DSR
VF0=YEP-YSP
TEM=9
NPR
ASD
YEP=YSP+VF0
DSD
OMD
HIT 'RETURN' TO CONTINUE
PAU
NPR
ASS
DSS
OMD
HIT 'RETURN' TO CONTINUE
PAU
TEM=5
NPR
XSP=XSP+VF1
XEP=XEP+VF1
END


!DCP
OMD
"DCP" COMPARES SEVERAL SPECTRA WHICH HAVE BEEN SCALED SO THAT A
OMD
SPECIFIED REF PEAK HAS THE SAME SCREEN HEIGHT IN ALL SPECTRA.
```

```
OMD
*
OMD
# OF FILES TO BE COMPARED:
VI0
OMD
CM-1 LIMITS FOR THE AUTOSCALING REFERENCE PEAK:
VF0
VF1
OMD
# OF CM-1 RANGES TO BE DISPLAYED:
QIT
FOR AAA=1 TIL QIT
OMD
ENTER A PAIR OF CM-1 RANGE LIMITS:
XSP
XEP
VF2=XSP
VF3=XEP
FOR III=1 TIL VI0
OMD
FILE #:
DFN
CSN=DFN
XSP=VF0
XEP=VF1
ASD
XSP=VF2
XEP=VF3
YSP=0
DSD
OMD
SHIFT THE BASELINE IF NECESSARY; THEN HIT "RETURN."
PAU
TEM=9
NPR
DFN=CSN
NXT III
TEM=5
NPR
NXT AAA
END


!DER
OMD
"DER" DERESOLVES AN ABSORBANCE FILE TO 16 CM-1 RESOLUTION
OMD
*
PFN=49
SPF
OMD
```

```
# OF FILE TO BE DERESOLVED:
DFN
ASD
DSD
TEM=9
NPR
NTP=2048
PTS=5
GFN
RESOLU.FTN
OFN=DFN
FRN
DSD
RPF
END


!DSC
DUM. "DSC" > DS1
DUM. COMPARES SUCCESSIVE FRAGMENTS OF 2 FILES USING CONSTANT
DUM. ABS/INCH.
DUM. YSP IS OBTAINED SEPARATELY FOR RFN & DFN BY AUTOSCALING.
DUM. YEP IS OBTAINED FOR RFN BY AUTOSCALING; & FOR DFN BY
DUM. ADDING THE RANGE OF RFN TO THE YSP OF DFN.
OMD
AUTO-SCALED (RFN) & COMPARISON (DFN) FILES:
RFN
DFN
OMD
STARTING CM-1 TO BE DISPLAYED:
XSP
OMD
CM-1 RANGE PER DISPLAY (- FOR DECREASING CM-1):
VF1
XEP=XSP+VF1
OMD
# OF DISPLAY RANGES:
QIT
TEM=9
FOR III=1 TIL QIT
DS1
NXT III
XSP=XSP-VF1
XEP=XEP-VF1
END


!DS1
DUM. "DS1"<DSC
ASR
DSR
```

```
VF0=YEP-YSP
TEM=9
NPR
ASD
YEP=YSP+VF0
DSD
OMD
HIT 'RETURN' TO CONTINUE
PAU
TEM=5
NPR
XSP=XSP+VF1
XEP=XEP+VF1
END


!DUM
END


!EMP
DUM. "EMP" > M99
OMD
"EMP" COPIES A SPECTRAL FILE INTO ALL VACANT FILES IN A BLOCK
OMD
OF SCRATCH FILES.  THIS PREVENTS AN 'INVALID FSB' MESSAGE FROM
OMD
OCCURRING DURING EXECUTION OF MACRO "TTL".
OMD
*
OMD
FILE TO BE COPIED:
OFN
OMD
1ST (SRT) & LAST (QIT) FILE #'S OF BLOCK:
SRT
QIT
DFN=SRT-1
FOR III=SRT TIL QIT
DFN=DFN+1
GFN
EMPFIL.FCP
FRN
CMR
NXT III
END


!FSP
OMD
```

```
*** "FSP" PRINTS A SECTOR OF FTIR SCRATCH FILE DATA ***
DUM. TO PRINT THE FILE STATUS BLOCK, REQUEST SECTOR FSZ/512
OMD
ENTER FILE #:
DFN
OMD
ENTER SECTOR # (HERE, THE 1ST SECTOR IS CALLED #1, NOT #0):
PTS
GFN
FSPRN.FCP
FRN
END



!FSW
DUM. "FSW" WRITES A WORD INTO THE STATUS BLOCK OF AN FTIR FILE
OMD
ENTER FILE #:
DFN
PAD
OMD
ENTER WORD # (HERE, THE WORD IS CALLED #1, NOT #0):
VI0
OMD
ENTER NEW VALUE OF WORD:
VI1
GFN
FSWR.FCP
FRN
END



!ITG
OMD
"ITG" INTEGRATES SELECTED CM-1 RANGES OF AN ABSORBANCE FILE.
OMD
SEE DIRECTIONS IN "INTGRL.FOR" FOR SETUP OF THE "INTSEG.DAT"
OMD
NICOS INPUT DATA FILE.
OMD
*
BAS=YS
GFN
INTGRL.FCP
OMD
DATA SET # OF "INTSEG.DAT":
VI2
OMD
NUMBER OF FILES:
VI0
OMD
```

```
INITIAL (VI3) & FINAL (QIT) CM-1 RANGE INDICES:
VI3=1
VI3
QIT
QIT=QIT+1
OMD
REFERENCE CM-1 RANGE INDEX:
VI1
OFN=VI1
FOR FFF=1 TIL VI0
OMD
INPUT FILE #:
DFN
TEM=4
NPR
TIQ
VI1=VI3-1
FRN
SMD
VF0=FCD
FOR III=VI3 TIL QIT
VI1=VI1+1
FRN
SMD
NXT III
TEM=4
NPR
NXT FFF
END


!LBB
OMD
"LBB" AUTO-TITLES A BLOCK OF SCRATCH FILES & TRANSMITS IT TO A
OMD
USER-SPECIFIED DISK LOCATION.
OMD
*
LB1
OMD
CM-1 RANGE TO BE SAVED (FXF, LXF):
FXF
LXF
DUM. SRT USED IN AUTIT.FCP
SRT=DFN
DFN=SRT-1
OMD
GENERIC FILE TITLE (SEE "ATG" MACRO FOR SPECIAL TITLE OPTIONS):
IMD
DFN=SRT
RTN=0
FOR AAA=1 TIL QIT
```

```
PRN DFN
GFN
AUTIT.FCP
FRN
TIQ
DFN=DFN+1
NXT AAA
DFN=SRT
OMD
OUTPUT FILES: NAME, DUMMY EXT, DEVICE, & DIR
OMD
E.G. ABS.000-D1[DATA]:
OMD
*
IFN
OMD
1ST EXTENSION # FOR OUTPUT:
EXT
FOR AAA=1 TIL QIT
PRN DFN
TIQ
ASP
EXT=EXT+1
DFN=DFN+1
NXT AAA
DFN=DFN-1
END



!LBI
DUM. "LBI" > LB1,LB2
OMD
*
OMD
"LBI" MOVES A BLOCK OF "I.EXT[,IRDATA]" INTERFEROGRAM FILES
OMD
CREATED BY MACROS "BAK", "STI", OR "SAM" TO A USER-SPECIFIED
OMD
LOCATION AFTER INITIALLY TRANSFERRI     EM TO A BLOCK OF FTIR
OMD
FILES.
OMD
*
GFN
I.000[,IRDATA
OMD
1ST EXTENSION # OF "I.EXT" FILES:
EXT
LB1
OFN=DFN
FOR III=1 TIL QIT
PRN DFN
```

```
AFG
DFN=DFN+1
EXT=EXT+1
NXT III
DFN=OFN
TIQ
PAD
FXI=0
LXI=NDP
LB2
END


!LBM
DUM. "LBM" > LB1,LB2
OMD
*
OMD
"LBM" COPIES A BLOCK OF SCRATCH FILES TO A USER-SPECIFIED DISK
OMD
LOCATION
OMD
*
LB1
OMD
CM-1 RANGE TO BE SAVED (FXF, LXF):
FXF
LXF
OMD
*
TIQ
LB2
END


!LBW
DUM. "LBW" > LB1,LB2
OMD
*
OMD
"LBW" COPIES A BLOCK OF WAVELENGTH FILES TO A USER-SPECIFIED
OMD
DISK LOCATION.
OMD
*
LB1
OMD
WAVELENGTH RANGE TO BE SAVED (FXL, LXL):
FXL
LXL
OMD
```

```
*
TIQ
LB2
END


!LB1
DUM. "LB1" < LBI & LBM
OMD
# OF FILES:
QIT
OMD
1ST SEQUENTIAL SCRATCH FILE:
DFN
END


!LB2
DUM. "LB2" < LBI & LBM
OMD
*
OMD
OUTPUT FILES: NAME, DUMMY EXT, DEVICE, & DIR
OMD
E.G. ABS.000-D1[DATA]:
OMD
*
IFN
OMD
1ST EXTENSION # FOR OUTPUT:
EXT
FOR III=1 TIL QIT
PRN DFN
TIQ
ASP
DFN=DFN+1
EXT=EXT+1
NXT III
END


!LTR
OMD
"LTR" TRANSMITS TEXT FROM THE KEYBOARD TO THE PLOTTER.  THE SIZE
OMD
& ORIENTATION OF THE LETTERS ARE USER SPECIFIED.
OMD
*
GFN
LETTRS.FCP
```

```
FRN
END


!MMM
END


!MMP
END


!M00
END


!M12
DUM. "M12" < SAM,STI
OMD
MINUTES FROM FINISH OF DATA CRUNCH TO START OF NEXT SCAN:
VI2
VI0=VI2*30
END


!M13
DUM. "M13" < SAM,STI
OMD
* * * * * * * * * DELAY IN PROGRESS * * * * * * * * *
DCL=212234
DCX
TEM=11
NPR
DCL=208138
DCX
END


!M14
DUM. "M14" < SAM,STI
END


!M15
DUM. "M15" < SAM,STI
OMD
```

```
HIT "RETURN" KEY WHEN READY TO CONTINUE.
PAU
END


!M17
DUM. "M17" < SA0 < BAK,SAM,STI,ALN
PFN=CSN
GFN
BENPAR.740
APG
RPF
END


!M19
DUM. "M19" < ALN
NSS=1
CLS
END


!M20
DUM. "M20" < BSL
OMD
ABSORBANCE INPUT FILE:
RFN
OMD
OUTPUT FILES FOR ABSORBANCE (DFN) & BASELINE PT DISPLAY (OFN):
DFN
OFN
OMD
1ST & LAST CM-1 OF CORRECTION RANGE:
FXF
LXF
END


!M21
DUM. "M21" < BSL
OMD
# OF DATA PTS PER BASELINE PT:
VI0=128
VI0
OMD
CM-1 RANGE LIMITS TO SKIP: (DSK,ITR), (RTN,PTS), (NTR,PEK).
OMD
SET UNUSED LIMITS TO ZERO:
DSK=0
```

```
DSK
ITR=0
ITR
RTN=0
RTN
PTS=0
PTS
NTR=0
NTR
PEK=0
PEK
END


!M23
DUM. "M23" < STI
OMD
FILE TITLE:
TID
END


!M30
DUM. "M30" < PLC
OMD
# OF INCHES OF Y-AXIS DEAD-SPACE BETWEEN PLOTS:
VF4=0.2
VF4
CMP=VI2/2
VF4=CMP*.01*SRM*VI2+VF4
PRN VF4
END


!M31
DUM. "M31" < PLC
OMD
Y-AXIS BASELINE OFFSET BETWEEN PLOTS (INCHES):
VF4
END


!M40
DUM  PLC & PLI > "M40" (SET ANGLES FOR A NONROTATED PLOT)
DUM. ANGLES OF X (SRT) & Y (RTN) AXES:
SRT=0
RTN=270
DUM. ANGLES OF X (FCD) & Y (RTO) TIC LABELS:
```

```
FCD=0
RTO=0
DUM. ANGLES OF X (XSL) & Y (YSL) AXIS NAMES:
XSL=0
YSL=90
END


!M41
DUM. PLC & PLI > "M41" (SET ANGLES FOR A ROTATED PLOT)
DUM.
DUM.              TEP LYT FXL SRT RTN FCD RTO XSL YSL
DUM. NORM ROT:     -   -   +   90   0  90 180  90 180
DUM. ANTI ROT:     +   +   -  270 180 270 270 270   0
DUM.
DUM. NORM ROT CAUSES "LINE" SUBROUTINE TO FAIL.
DUM.
DUM. ANGLES OF X (SRT) & Y (RTN) AXES:
SRT=270
RTN=180
DUM. ANGLES OF X (FCD) & Y (RTO) TIC LABELS:
FCD=270
RTO=270
DUM. ANGLES OF X (XSL) & Y (YSL) AXIS NAMES:
XSL=270
YSL=0
DUM. X AXIS IS IN - DIRECTION FOR A ROTATED PLOT:
¯XL=-FXL
END


!M42
DUM. "M42" < PLC, PLI
ASD
DSD
OMD
1ST & LAST Y AXIS LIMITS:
YSP
YEP
OMD
1ST TIC LABEL ON Y AXIS:
FYI
OMD
TIC LABEL SPACING FOR Y AXIS:
CYA
END


!M43
DUM. "M43" < PLC, PLI
```

```
RFN=DFN
ASR
END


!M44
DUM. "M44" < PLC, PLI
RFN=SMN
ASR
END


!M45
DUM. "M45" < PLC, PLI
OMD
AUTOSCALE LIMITS FOR X AXIS:
XSP
XEP
WTY=-15
END


!M46
DUM. PLC & PLI > "M46" (SCALE PARAMETERS) > M45
OMD
1ST & LAST X VALUES TO BE PLOTTED:
FXF
LXF
XSP=FXF
XEP=LXF
OMD
1ST TIC LABEL ON X AXIS:
LXI
OMD
SPACING OF TIC LABELS ON X AXIS:
CXL
OMD
LENGTHS (INCHES) OF X (FXL) & Y (LYT) AXES:
FXL
LYT
OMD
AUTOSCALING: 0=NONE, 1=ALL, >1 = AUTOSCALE ONCE USING FILE SMN
SMN=1
SMN
DUM: CALL M45 (AUTOSCALE LIMITS) OR MMM (NOTHING)
CMP=SMN/10000
CMP=46*CMP-1
CMR
DUM. MARGIN (1/100 INCHES) BETWEEN AUTOSCALED SPECTRUM BASELINE
DUM. & X AXIS:
```

```
MNT=10
END


!M47
DUM. PLC & PLI > "M47" (MISC INPUT PARAMETERS > (M30-31)
OMD
# OF PLOTS:
QIT
OMD
PLOT TITLES (0=NO, 1=YES)?  NOTE: TITLE OFFSET = PLOT OFFSET
VI2
OMD
INITIAL PEN # FOR SPECTRAL DATA:
PEK=1
PEK
OMD
SPECTRUM PEN # INCREMENT FOR SUCCESSIVE PLOTS:
NSS=0
NSS
OMD
OVERLAP Y-AXES (0=NO, 1=YES)?
OFN=OFN/10000
OFN
OFN=OFN/10000
CMP=OFN+30
CMR
END


!M48
DUM. PLC & PLI > "M48" > (M40,41)
OMD
ROTATE PLOT (0=NO, 1=YS)?
RTR=RTR/10000
RTR
OMD
ORIGIN (INCHES) OF X (LXL) & Y (LYA) AXES VS. ZPN:
OMD
      (NOTE:    FOR A ROTATED PLOT, LXL ~ 1 + X-AXIS LENGTH)
LXL=FXL*RTR+1
LXL
LYA
CMP=RTR/10000+40
CMR
OMD
# RATIO OF MINOR TO MAJOR TICS:
RTP
GFN
PLPARW.FCP
FRN
```

```
END


!M49
DUM. PLC & PLI > "M49"
GFN
PLPARR.FCP
FRN
END


!M50
DUM. SA5 < "M50" < SAM,STI
BFN
PAB
OMD
DETECTOR:
DET
OMD
APERTURE (SM, MD, OR FL)
APT
OMD
ENTER 12 FOR AUTO-TIMED SPECTRA; 14 FOR MANUAL:
VI1
CMP=VI1
CMR
OMD
# OF SCANS PER SPECTRUM:
NSD
OMD
# OF SPECTRA TO BE COLLECTED
QIT
SA5
END


!M51
DUM. "M51" < SAM
BFN=3
PRN BFN
PAB
DET=1
PRN DET
APT=MD
PRN APT
VI1=12
OMD
PROGRAM PAUSE (MIN) BETWEEN AUTO-SCANS:
VI2=60
PRN VI2
```

```
VI0=VI2*30
OMD
SCANS PER SPECTRUM:
NSD=500
PRN NSD
OMD
# OF SPECTRA TO BE COLLECTED:
QIT=20
PRN QIT
OMD
1ST & LAST CM-1 FOR 1ST DISPLAY:
VF0=4000
VF1=600
PRN VF0
PRN VF1
OMD
1ST & LAST CM-1 FOR 2ND DISPLAY:
VF2=1200
VF3=1650
PRN VF2
PRN VF3
END


!M52
DUM. "M52" < SAM,STI
BFN=3
PRN BFN
PAB
DET=1
PRN DET
APT=MD
PRN APT
VI1=14
OMD
SCANS PER SPECTRUM:
NSD=100
PRN NSD
OMD
# OF SPECTRA TO BE COLLECTED:
QIT=40
PRN QIT
OMD
1ST & LAST CM-1 FOR 1ST DISPLAY:
VF0=4000
VF1=600
PRN VF0
PRN VF1
OMD
1ST & LAST CM-1 FOR 2ND DISPLAY:
VF2=1200
VF3=1700
```

```
PRN VF2
PRN VF3
END


!M99
DUM. "M99" < EMP
MOD
END


!NSF
OMD
*** "NSF" COPIES A BLOCK OF FILES FROM NICOS TO FTIR ***
OMD
*
OMD
GENERIC FILE NAME & LOCATION:
OMD
E.G.    FILNAM    OR    FILNAM[DIR]    OR    FILNAM.000-D1[DIR]
IFN
OMD
1ST EXTENSION #:
EXT
OMD
1ST SCRATCH FILE #:
DFN
OMD
# OF FILES TO COPY:
QIT
FOR III=1 TIL QIT
PRN DFN
AFG
DFN=DFN+1
EXT=EXT+1
NXT III
DFN=DFN-1
END


!NXP
OMD
NEXT PAGE ADVANCE FOR ZETA-8 PLOTTER
SF2=RO
YPN=-8.5
XPN=0
PEN
YPN=0
ZPN
SF2=BT
```

```
END


!PCP
DUM: "PCP" > PC1
PC1
OMD
1) SET PEN AT PERFORATION; 2) [CR]
PAU
XPN=1
YPN=1
PEN
FOR AAA=1 TIL QIT
DFN=VI1-1
ZPN
AXS=XO
OMD
PLOTTING RANGE:
FXF
LXF
OMD
CM-1 PER INCH (NEG IF FXF>LXF ):
CXF
FXL=LXF-FXF
FXL=FXL/CXF
FOR III=1 TIL VI0
DFN=DFN+1
XSP=VF0
XEP=VF1
ASD
YSP=0.0
YEP=YEP/VF3
CYA=YEP/VF2
XSP=FXF
XEP=LXF
DSD
OMD
1) USE CURSOR TO RAISE BASELINE FULLY INTO VIEW; 2) [CR]
PAU
TEM=9
NPR
FYA=YSP
LYA=YEP
TEM=103
NPR
PLD
PCL=CSN+PCL
TEM=100
NPR
XPN=0
YPN=VF4
PEN
```

```
AXS=NO
NXT III
PCL=0
PL6
TEM=5
NPR
NXT AAA
END


!PC1
DUM: "PC1" < PCP
OMD
"PCP" COMPARES A BLOCK OF SPECTRA BY EQUALIZING THE ABSORBANCES
OMD
OF A SELECTED BAND.  MULTIPLE CM-1 RANGES CAN BE SPECIFIED.
OMD
*
OMD
AUTOSCALE LIMITS FOR REFERENCE BAND (XSP, XEP):
XSP
XEP
VF0=XSP
VF1=XEP
OMD
RATIO OF AUTOSCALED PEAK ABSORBANCE TO YEP:
VF3
OMD
TITLES (YS OR NO)?
TIT
OMD
AUTO PEN CHANGE (0=NO, 1=YS)?
CSN=0
CSN
OMD
# OF CM-1 RANGES TO BE PLOTTED:
QIT
OMD
TOTAL # OF SEQUENTIAL SCRATCH FILES:
VI0
OMD
Y-AXIS OFFSET BETWEEN PLOTS:
VF4=1
VF4
VF2=10-VI0
OMD
1ST FILE #:
VI1
SF2=NO
RTR=0
LYT=0
END
```

```
!PFB
DUM. "PFB" < R#W & M17(ALN,BAK,STI,SAM)
DUM. "PFB" READS PARAMETER FILE PFN OF "BENPAR.740"
GFN
BENPAR.740
APG
RPF
PRN NDP
PRN NTP
PRN FSZ
PRN MIR
PRN LPS
PRN HPS
PRN VEL
PRN XSP
PRN XEP
PRN SFN
PRN BFN
PRN DFN
PRN RFN
PRN NSS
PRN NSB
PRN NSD
PRN APT
PRN DET
END


!PLC
DUM: "PLC" > PL1-PL4,PL7,M(30-31,40-49)
OMD
"PLC" COMPARES SEVERAL PLOTS ON 1 X-AXIS ***********
PFN=49
SPF
TEM=100
NPR
PL1: DEFAULT TITLE   PARAMETERS
PL2:      "   AXES         "
PL3:      "    TIC         "
PL4:      "   TIC LABEL    "
OMD
NICOS (0) OR MANUAL (1) INPUT ?
BFN=BFN/1000
BFN
BFN=BFN/1000
CMP=51*BFN-5
DUM: SET SCALE PARAMS (M46 OR MMM)
CMR
CMP=51*BFN-4
DUM: MISC INPUT (M47 OR MMM)
```

```
CMR
CMF=51*BFN-3
DUM: MISC INPUT (M48 OR MMM)
CMR
CMP=51*BFN+49
DUM: READ "PLT.DAT" PARAMS; (M49 OR MMP)
CMR
PL7: PLOTTING LOOP.
PFN=49
RPF
END



!PLI
DUM: "PLI" > PL1-PL6,M(40-46,48,49)
OMD
*** "PLI" PLOTS N FILES ON N X-AXES ***
OMD
WAIT FOR PROMPTS
PFN=49
SPF
TEM=100
NPR
PL1: DEFAULT TITLE   PARAMETERS
PL2:      "    AXES        "
PL3:      "    TIC         "
PL4:      "   TIC LABEL    "
OMD
NICOS (0) OR MANUAL (1) INPUT ?
BFN=BFN/1000
BFN
BFN=BFN/1000
CMP=51*BFN-5
DUM: SET SCALE PARAMS (M46 OR MMM)
CMR
CMP=51*BFN-3
DUM: MISC INPUT (M48 OR MMM)
CMR
CMP=51*BFN+49
DUM: READ "PLT.DAT" PARAMS; (M49 OR MMP)
CMR
PL5: PLOTTING LOOP.
PFN=49
RPF
END



!PL1
DUM  PLC & PLI > "PL1" (DEFAULT TITLE PARAMETERS)
DUM.  PLOT TITLE (0=NO, 1=YES, 2=USE MACRO DESCRIPTOR AS TITLE)?
VI2=1
```

```
DUM. INCHES FROM ORIGIN OF X AXIS TO 1ST LETTER OF TITLE
DUM. MEASURED ALONG X AXIS (NEGATIVE # GIVES AUTO-CENTERING):
FXI=0
DUM. INCHES FROM UPPER LIMIT OF Y AXIS TO 1ST LETTER OF TITLE
DUM. MEASURED ALONG Y AXIS:
LYE=0.1
DUM. SIZE OF TITLE LETTERS IN 1/100 INCHES:
SRM=15
DUM. PEN # FOR TITLE:
VI3=1
END



!PL2
DUM. PLC & PLI > "PL2" (DEFAULT AXES PARAMETERS)
DUM. PLOT X AXIS (0=NO, 1=YES)?
VI0=1
DUM. PLOT Y AXIS (0=NO, 1=YES)?
VI1=1
DUM. SIZE OF LETTERS OF AXES NAMES IN 1/100 INCHES (A NEGATIVE
DUM. VALUE KILLS THE AXES NAMES):
SRN=15
DUM. PEN # FOR AXES:
PTS=1
END



!PL3
DUM. PLC & PLI > "PL3" (DEFAULT TIC PARAMETERS)
DUM. MAJOR TIC SIZE IN 1/100 INCHES:
DSK=10
DUM. SIZE RATIO OF MAJOR TO MINOR TICS:
FCB=2.0
DUM. # RATIO OF MINOR TO MAJOR TICS FOR X (RTP) & Y (RTQ) AXES:
RTP=1
RTQ=0
DUM. MARGIN (1/100 INCHES) BETWEEN TIC LABELS & TICS:
SIZ=10
DUM. MARGIN (1/100 INCHES) BETWEEN TIC LABELS & AXIS NAME:
NSR=20
END



!PL4
DUM. PLC & PLI > "PL4" (DEFAULT TIC LABEL PARAMETERS)
DUM. DIGIT SIZE (1/100 INCHES) FOR X (ITR) & Y (WTY) TIC
DUM. LABELS; - SIGN KILLS TICS & TIC LABELS:
ITR=15
WTY=15
DUM. IF TIC LABEL & AXIS ARE PARALLEL, GIVE # OF CHARACTERS OF
```

```
DUM. TIC LABEL TO LIE TO THE RIGHT OF THE X (VF2) OR Y (VF3)
DUM. TIC MARK.
VF2=1.6
VF3=1.6
DUM. # OF DIGITS TO RIGHT OF DECIMAL POINT FOR X (NTR) & Y (PFN)
DUM. AXES; PFN > 10 GIVES AUTO-CALCULATED VALUE FOR Y AXIS:
NTR=0
PFN=11
END



!PL5
DUM. PLI > "PL5" > M42-44
DUM: SET Y-AXIS MACRO (M42, M43, OR M44)
CMP=SMN+9999
CMP=CMP/10000-1
CMP=SMN/10000+CMP+42
OMD
TITLES (0=NO, 1=YES)?
VI2
DUM. TURN OFF OVERLAP PARAMETERS (OFN & VF4):
OFN=0
VF4=-11
OMD
# OF PLOTS:
QIT
ZPN
PAU SET PEN AT PERFORATION <CR>
FOR III=1 TIL QIT
PEK=1
OMD
FILE #:
DFN
PAD
ZPN
ASD
DSD
CMR
GFN
PLOTFT.FCP
FRN
PL6
NXT III
END



!PL6
DUM. "PL6" < PLI & PCP  *** SET NEW PAGE ON PLOTTER ***
DUM. FXL & LYT ARE THE X AND Y AXIS LENGTHS, RESPECTIVELY.
DUM. RTR DENOTES NONROTATED (0) OR ROTATED (1) PLOT.
DUM. INITIALLY, XPN & YPN ARE USED AS TEMPORARY JUNK VARIABLES.
```

```
XPN=FXL+.1
YPN=1-RTR
YPN=YPN*XPN/8.5
XPN=LYT+.1
XPN=RTR*XPN/8.5
DUM. PEK IS THE TRUNCATED INTEGER SUM OF REAL #'S
PEK=XPN+YPN
XPN=8.5*PEK
YPN=0
PEN
END


!PL7
DUM. PLC > "PL7" > (M42-44)
DUM: SET Y-AXIS MACRO (M42, M43, OR M44)
CMP=SMN+9999
CMP=CMP/10000-1
CMP=SMN/10000+CMP+42
ZPN
SFN=SMN/10000
DTD=0
DUM.
DUM. *** BEGIN PLOTTING LOOP ***
DUM.
FOR AAA=1 TIL QIT
OMD
FILE # FOR PLOT:
DFN
PAD
PLO=300
VI3=PEK
DUM. SET Y SCALE:
CMR
GFN
PLOTFT.FCP
FRN
DUM. AXES(VI0,VI1) & Y-INPUT(CMP) ON/OFF:
VI0=0
VI1=1-OFN
CMP=SFN*CMP
DTD=DTD+1
PEK=PEK+NSS
NXT AAA
END


!PMY
OMD
*** "PMY" PRINTS Y-AXIS LIMITS FOR A BLOCK OF FTIR FILES ***
OMD
```

```
1ST FILE #:
SRT
OMD
LAST FILE #:
QIT
DFN=SRT
DUM: USE SUB-BLOCKS OF SIZE RTN FOR SCREEN DISPLAY:
RTN=8
RTO=1
VI1=QIT-SRT+1
VI2=VI1
VI3=VI2/RTN
FOR III=1 TIL VI3
DUM: CALC UPPER INDEX (RTQ) FOR SUB-BLOCK:
RTO=RTO+1
RTP=RTO/VI3
RTP=2-RTP
RTQ=1-RTP
RTP=RTN*RTP
RTQ=VI2*RTQ+RTP
FOR JJJ=1 TIL RTQ
OMD
**************
ASD
DSD
PRN DFN
PRN YSP
PRN YEP
DFN=DFN+1
NXT JJJ
VI2=VI2-RTN
OMD
**************
PAU/ TYPE [CR] TO CONTINUE
NXT III
END


!PPP
DUM. "PPP" > PP1
OMD
"PPP" PLOTS & PEAK-PICKS AN FTIR SCRATCH FILE
PP1
OMD
FILE #:
DFN
ASD
DSD
OMD
1ST & LAST Y-AXIS VALUES:
FYA
LYA
```

```
OMD
ABSORBANCE UNITS PER INCH:
CYA
OMD
PPK THRESHOLD VALUE:
THR
OMD
AXIS OPTION (YS, NO, XO):
AXS
OMD
1) SET PEN AT NEAR (SF2=NO) OR FAR (SF2=RO) PAPER PERFORATION
OMD
2) [CR]
PAU
ZPN
PEN
TEM=103
NPR
PLP
XPN=0-XPN
YPN=0-YPN
PEN
TEM=100
NPR
YPN=1
XPN=0-XPN
END



!PP1
DUM. "PP1" < PPP
TEM=100
NPR
PLO=0
FIT=YS
TIT=NO
PUP=YS
OMD
1ST & LAST CM-1 (NOTE: AXIS LENGTH MUST BE AN INTEGER):
FXF
LXF
XSP=FXF
XEP=LXF
OMD
CM-1 PER INCH (NEGATIVE FOR FXF>LXF):
CXF
OMD
SMOOTHING OPTION (YS, NO):
SMO
OMD
RESET 'PTS' IF SMOOTHING IS DESIRED (ALLOWED VALUES = 3-25)
PTS=3
```

```
PTS
OMD
PLOT ROTATION? (RO, NO):
SF2
OMD
SHIFTS (INCHES) IN THE X-AXIS (XPN) & Y-AXIS (YPN)
OMD
ORIGINS VS THE ZPN POINT:
XPN
YPN
END



!PR1
GFN
PARAM1.GCP
FRN
END



!PR2
GFN
PARAM2.GCP
FRN
END



!PR3
GFN
PARAM3.GCP
FRN
END



!PR4
GFN
PARAM4.GCP
FRN
END



!PR5
GFN
PARAM5.GCP
FRN
END
```

```
!RES
OMD
*** "RES" CHANGES THE RESOLUTION OF AN ABSORBANCE FILE ***
OMD
INPUT FILE #:
OFN
OMD
OUTPUT FILE #:
DFN
OMD
RESOLUTION OF OUTPUT FILE (CM-1):
VF1
NTP=32768/VF1
PRN NTP
GFN
RESOLU.FTN
FRN
END


!R0W
DUM. "R0W" > PFB
OMD
SETTING RESOLUTION TO 0.5 CM-1
PFN=0
PFB
END


!R1W
DUM. "R1W" > PFB
OMD
SETTING RESOLUTION TO 1 CM-1
PFN=1
PFB
END


!R2W
DUM. "R2W" > PFB
OMD
SETTING RESOLUTION TO 2 CM-1
PFN=2
PFB
END
```

```
!R3W
DUM. "R3W" > PFB
OMD
SETTING RESOLUTION TO 0.3 CM-1
PFN=3
PFB
END



!R4W
DUM. "R4W" > PFB
OMD
SETTING RESOLUTION TO 4 CM-1
PFN=4
PFB
END



!SAM
DUM: "SAM" > SA(0,2-5,9),M(12-15,17,50-52)
OMD
*** "SAM" COLLECTS, DISPLAYS, & AUTO-TITLES SAMPLE SPECTRA ***
OMD
*
OMD
INPUT OPTION: 50 = KEYBOARD INPUT
OMD
              51 = AUTOSCAN WITH DEFAULT PARAMETERS FROM M51
OMD
              52 = MANUAL SCAN WITH DEFAULT PARAMETERS FROM M52
CMP=51
CMP
TEM=100
NPR
CMR
OMD
1ST SPECTRAL FILE # (FILE DFN-1 MUST HAVE VALID FSB):
DFN
DUM. SRT USED IN AUTIT.FCP
SRT=DFN
DFN=SRT-1
OMD
GENERIC FILE TITLE (SEE "ATG" MACRO FOR SPECIAL TITLE OPTIONS):
IMD
DFN=SRT
SFN=2
RTN=0
OMD
*
OMD
HIT "RETURN" TO START
```

```
PAU
SA2
END


!SA0
DUM.  M17 < "SA0" < BAK & SAM & STI & ALN
OMD
****************************
DUM: THE "SA0" MACRO SETS PFN=CSN (VIA "M17") IF PFN & CSN ARE
DUM: NOT EQUAL.  OTHERWISE, "SA0" DOES NOTHING.
CMP=PFN-CSN
CMP=CMP/100
MNT=CSN-PFN
CMP=MNT/100+CMP
CMP=18*CMP-CMP
CMR
END


!SA2
DUM. "SA2" < SAM,STI
FOR AAA=1 TIL QIT
SA3: COLLECT INTERFEROGRAM INTO DFN & COPY IT TO I.EXT[,IRDATA].
DUM: THEN TRANSFORM & DISPLAY DATA.
SA4: DISPLAY 1ST CM-1 RANGE OF CURRENT & PREVIOUS RFN.
OMD
FILE & STARTING TIME FOR MOST RECENTLY PROCESSED SPECTRUM:
PRN DFN
STD
CMP=23*RTN
CMR
CMP=VI1+1
DUM: AUTO-DELAY (M13) OR MANUAL PAUSE (M15).
CMR
DUM: RESET CM-1 LIMITS & CLEAR SCREEN.
XSP=VF2
XEP=VF3
TEM=5
NPR
ASD
SA4: DISPLAY 2ND CM-1 RANGE OF CURRENT & PREVIOUS SPECTRUM
CMR
DFN=DFN+1
NXT AAA
DFN=DFN-1
END


!SA3
```

```
DUM. "SA3" < SAM,STI
XSP=VF0
XEP=VF1
CLD
GFN
AUTIT.FCP
FRN
GFN
I.000[,IRDATA]
EXT=DFN
DUM: AFP OPERATES ON DFN.
AFP
FPD
OFN=DFN
MOS
RAD
ABD
ASD
END



!SA4
DUM. "SA4" < SAM,STI
RFN=DFN-1
DSR
TEM=9
NPR
DSD
END



!SA5
DUM. "SA5" < SAM,STI
VF0=4000
OMD
INITIAL & FINAL CM-1 FOR 1ST DISPLAY:
VF0
VF1
OMD
INITIAL & FINAL CM-1 FOR 2ND DISPLAY:
VF2
VF3
END



!SA6
DUM. M50-M52 < "SA6" < SAM,STI
SFN=2
OMD
```

```
*
OMD
1ST SPECTRAL FILE # (FILE DFN-1 MUST HAVE VALID FSB):
DFN
SRT=DFN
OMD
INPUT OPTION: 50 = KEYBOARD INPUT
OMD
              51 = AUTOSCAN WITH DEFAULT PARAMETERS FROM M51
OMD
              52 = MANUAL SCAN WITH DEFAULT PARAMETERS FROM M52
CMP=51
CMP
TEM=100
NPR
CMR
OMD
GENERIC FILE TITLE (SEE "ATG" MACRO FOR SPECIAL TITLE OPTIONS):
IMD
OMD
HIT "RETURN" TO START
PAU
END



!SA9
DUM: "SA9" < SAM & STI
DUM: ROUTING DOCUMENTATION FOR "SAM" MACRO:
DUM: SAM/STI     SET UP INPUT
DUM: SA2-4       COLLECT & DISPLAY SPECTRA
DUM: M12-13      MANUAL DELAY
DUM: M14         DUMMY CONDITIONAL MACRO
DUM: M15         AUTO   DELAY
DUM: M23         MANUAL TITLE
DUM: M50-SA5     KEYBOARD INPUT
DUM: M51 OR 52   DEFAULT    "
END



!SBS
DUM. "SBS" > SB1,SB0
OMD
"SBS" REGENERATES 1-BEAM FILE FROM ABSORBANCE & 2ND 1-BEAM.
TEM=100
NPR
PFN=49
SPF
SB0
SB1. CONVERT INPUT 1-BEAM (RFN) TO "AUTO-ABSORBANCE" (DFN).
DUM. SET DFN = OUTPUT FILE
DFN=1-CMP
```

```
DFN=DFN*SFN
DFN=CMP*BFN+DFN
MOD
DUM. SAMPLE "AUTO-ABS" = ABS + BG "AUTO-ABS"
OFN=1
FCO=1
FCD=-2*CMP+1
ADD
DUM. SET NSD = # SCANS FOR OUTPUT FILE
PAD
VI1=1-CMP
NSD=VI1*NSD
NSD=CMP*NSB+NSD
DUM. CONVERT SAMPLE TO %T, & RECLASSIFY AS 1-BEAM.
TXD
DUM. "FRN" RECLASSIFIES %T AS 1-BEAM & RESETS FCD.
FRN
OFN=DFN
VAL
FCD=FCD/FCO
MUD
ASD
DSD
RPF
END



!SB0
DUM. "SB0" < SBS
OMD
SAMPLE (SFN), BG (BFN), & ABSORBANCE (OFN) FILES:
SFN
BFN
OFN
OMD
REGENERATE SFN (CMP=0) OR BFN (CMP=1)?
CMP=0
CMP
OMD
CM-1 RANGE FOR SCREEN DISPLAY:
XSP
XEP
DUM. SET RFN = 1-BEAM INPUT FILE:
RFN=1-CMP
RFN=RFN*BFN
RFN=CMP*SFN+RFN
DUM. READ DATA VALUES AT XSP FOR BOTH INPUT FILES FOR CALC OF
DUM. OUTPUT FILE MULTIPLIER (VIA "SBFTYP.FCP").
VAL
VF0=FCO
VI2=OFN
OFN=RFN
```

```
VAL
VF1=FCO
OFN=VI2
DFN=1
END


!SB1
DUM. "SB1" <  SBS & AOB
DUM. CONVERT 1-BEAM FILE (RFN) TO "ABSORBANCE" (DFN) USING
DUM. THE MAX INTENSITY BETWEEN XSP & XEP AS THE "BACKGROUND"
DUM. FOR RFN.
RTN=DFN
RTO=BFN
BFN=RFN
DFN=0
MRD
RAD
DUM. FILE 0 IS NOW 100%T.  USE "SBFTYP.FCP" TO RECLASSIFY FILE 0
DUM. AS 1-BEAM WITH: "INTENSITY" = 1/NSR
GFN
SBFTYP.FCP
FRN
PAR
ASR
FCD=NSR*YEP
MUD
DUM. FILE 0 NOW EQUALS YEP FOR ALL CM-1; I.E. NSR*YEP*1/NSR=YEP
DFN=RTN
DUM. RATIO RFN TO RMAX (YEP CANCELS OUT)
MRD
BFN=0
RAD
ABD
BFN=RTO
END


!SMH
OMD
"SMH": ***** SPECTRUM SMOOTHING MACRO *****
OMD
INPUT (OFN) & OUTPUT (DFN) FILES:
OFN
DFN
OMD
# OF POINTS:
PTS
OMD
CM-1 RANGE:
XSP
```

```
XEP
OMD
DYNAMIC (YS) OR NORMAL (NO) SMOOTHING?
SMO
OMD
MINIMUM NOISE (%T):
THR
VIO=0
GFN
SMOOTH.FTN
FRN
END


!SMT
OMD
** "SMT" SMOOTHS A SPECTRUM & WRITES OUTPUT TO A NEW FILE **
OMD
FILE TO BE SMOOTHED:
SFN
PAS
OMD
OUTPUT FILE:
DFN
OMD
HALF-WIDTH AT HALF MAXIMUM (CM-1 OR WVL) OF SMOOTHING FUNCTION:
VFO
OMD
X-AXIS RANGE TO BE SMOOTHED:
XSP
XEP
MSD
TEM=4
NPR
GFN
SMT.FCP
FRN
ASD
DSD
NPR
END


!STI
DUM. "STI" > SA(0,2-6,9),M(12-15,17,23,50-52)
OMD
"STI" COLLECTS & DISPLAYS SAMPLE SPECTRA; IT PAUSES FOR KEYBOARD
OMD
INPUT OF A TITLE PRIOR TO EACH DATA COLLECTION.
OMD
*
```

```
SA6
RTN=1
SA2
END


!STK
OMD
"STK" GENERATES A STICK SPECTRUM FROM ABSORBANCE DATA IN NICOS
OMD
ASCII FILE "STICK.DAT".  SEE DIRECTIONS IN "STICK.FOR" FOR SETUP
OMD
OF "STICK.DAT".
OMD
*
OMD
SPECIFY A JUNK SCRATCH FILE THAT ALREADY CONTAINS ABSORBANCE
OMD
DATA.  THE STICK SPECTRUM WILL BE SENT TO THIS FILE.
DFN
TXD
OMD
ENTER DATA SET # OF NICOS FILE "STICK.DAT".
VI0
PAD
GFN
STICK.FCP
FRN
ABD
ASD
DSD
END

!SUM
OMD
*** "SUM" ADDS RFN TO DFN AS FOLLOWS:
OMD
*
OMD
  FCR * RFN + FCD * DFN + VF3 = OFN
OMD
*
OMD
VF3 IS AN ADDITIVE CONSTANT; OFN IS THE OUTPUT FILE
OMD
************************
OMD
CM-1 RANGE TO BE ADDED:
FXF
LXF
XSP=FXF
XEP=LXF
```

```
OMD
INPUT (RFN, DFN) & OUTPUT (OFN) FILE #'S:
RFN
DFN
OFN
OMD
SCALE FACTORS:
FCR
FCD
OMD
ADDITIVE CONSTANT:
VF3=0
VF3
PAD
SU0. CALL "SUMSPC.FCP"
SFN=OFN
ASS
DSS
END


!SU0
DUM. "SU0" < SUM
TEM=100
NPR
ASR
VF1=YEP
ASD
VF2=YEP
GFN
SUMSPC.FCP
FRN
END


!SVI
DUM: "SVI" > SV0-SV3
OMD
*** INTERACTIVE SUBTRACTION OF H2O & CO2 VAPOR ***
SV2
GFN
H2OA2.000[VAPOR
SV3
XSP=1700
XEP=1600
SV0
ASS
DSS
FCR=1
OMD
SET "FCR" NEGATIVE IF VAPOR PEAKS ARE NEGATIVE ON GREEN DISPLAY:
FCR
```

```
SV1
GFN
H2OA13.000[VAPOR
SV3
XSP=3800
XEP=3600
SV0
SV1
GFN
CO2A3.000[VAPOR
SV3
XSP=2400
XEP=2280
SV0
ASS
DSS
FCR=1
OMD
SET "FCR" NEGATIVE IF VAPOR PEAKS ARE NEGATIVE ON GREEN DISPLAY:
FCR
SV1
GFN
CO2A2.000[VAPOR
SV3
XSP=625
XEP=715
SV0
SV1
GFN
CO2A1.000[VAPOR
SV3
XSP=3760
XEP=3550
SV0
SV1
RPF
END

!SVP
DUM: "SVP" > SV0-SV3
OMD
*** INTERACTIVE SUBTRACTION OF H2O & CO2 VAPOR ***
OMD
"SVP" USES THE SAME MULTIPLIER FOR ALL BANDS OF A GIVEN VAPOR.
OMD
USE "SVI" IF INDIVIDUAL MULTIPLIERS ARE DESIRED.
SV2
GFN
WAT123.000[VAPOR
SV3
XSP=1700
XEP=1600
SV0
```

```
ASS
DSS
FCR=1
OMD
SET "FCR" NEGATIVE IF VAPOR PEAKS ARE NEGATIVE ON GREEN DISPLAY:
FCR
SV1
GFN
CD123.000[VAPOR
SV3
XSP=2400
XEP=2280
SV0
ASS
DSS
FCR=1
OMD
SET "FCR" NEGATIVE IF VAPOR PEAKS ARE NEGATIVE ON GREEN DISPLAY:
FCR
SV1
RPF
END


!SV0
DUM: "SV0" < SVI & SVP
DUM: DISPLAY VAPOR SPECTRUM & FREEZE IT
ASR
DSR
TEM=9
NPR
END


!SV1
DUM: "SV1" < SVI & SVP
OMD
*
OMD
1) DO INTERACTIVE SUBTRACTION USING X-ZOOM KEYS
OMD
2) USE <CNTRL E> TO SAVE SUBTRACTION; OTHERWISE GO TO STEP #3
OMD
3) USE <CR> TO RESUME MACRO:
SUB
PAU
TEM=5
NPR
END
```

```
!SV2
DUM: "SV2" < SVI & SVP
OMD
*
OMD
REFERENCE VAPOR SPECTRA ARE ASSUMED TO BE IN DIRECTORY [VAPOR].
OMD
THE FILE EXTENSIONS DENOTE RESOLUTION (E.G. EXT=002 FOR 2 CM-1).
OMD
*
DUM: SYSTEM MACRO "SUB" SUBTRACTS RFN FROM SFN; "SV2" PUTS
DUM: RFN=1, & SETS DFN=RFN SO THAT "AFG" CAN RETRIEVE THE
DUM: 1ST VAPOR SPECTRUM INTO FILE 1.
OMD
FILE # FOR VAPOR-CONTAMINATED ABSORBANCE SPECTRUM:
SFN
PFN=49
SPF
PAS
RFN=1
DFN=1
FCR=1
END


!SV3
DUM: "SV3" < SVI & SVP
DUM: EXT=0 FOR 0.5 CM-1 RES; 2 FOR 2 CM-1.
EXT=32769/NTP-1
AFG
END


!TTL
OMD
*** "TTL" PRINTS A BLOCK OF FTIR FILE TITLES & START TIMES ***
OMD
1ST FILE #:
VI0
OMD
LAST FILE #:
QIT
DFN=VI0
DUM: USE SUB-BLOCKS OF SIZE RTN FOR SCREEN DISPLAY:
RTN=8
RTO=1
VI1=QIT-VI0+1
VI2=VI1
VI3=VI2/RTN
FOR III=1 TIL VI3
```

```
DUM: CALC UPPER INDEX (RTQ) FOR SUB-BLOCK:
RTO=RTO+1
RTP=RTO/VI3
RTP=2-RTP
RTQ=1-RTP
RTP=RTN*RTP
RTQ=VI2*RTQ+RTP
FOR JJJ=1 TIL RTQ
OMD
**************
PRN DFN
TIQ
STD
DFN=DFN+1
NXT JJJ
VI2=VI2-RTN
OMD
**************
PAU/ TYPE [CR] TO CONTINUE
NXT III
END


!UVV
OMD
*** "UVV" COPIES UV-VIS DATA FROM A USER-SPECIFIED NICOS FILE TO
OMD
A BLOCK OF FTIR FILES.  THE UV-VIS DATA ARE OBTAINED BY INTER-
OMD
COMPUTER TRANSFER: SND.OY (PE-7500) > PDAPAK.FOR (ZENITH) >
OMD
XMODEM (NICOLET).
OMD
*
OMD
# OF FILES:
QIT
OMD
1ST FILE:
DFN
OMD
NICOS FILE NAME & DIRECTORY:
TID
GFN
UVVIS.FCP
FRN
XSP=190
XEP=900
ASD
DSD
END
```

```
C ------------------------------------------------------------
C "AMAC.FOR"
C
C CALLS:  "SORT.FOR"
C ------------------------------------------------------------
C
      PROGRAM AMAC
      INTEGER*2 ISIZE
      INTEGER ISORT(200),NAM(3)
      REAL CODE(200)
      CHARACTER CHR(64)*1, BLANK*1,GEN*6,EX(10)*2,FILNAM*8,
     $          CONC*64,EOF*2,CHRS*64,TRIM*64
      DATA BLANK/' '/,
     $     EX/'0\','1\','2\','3\','4\','5\','6\','7\','8\','9\'/
     $     ,GEN/'JUNK.\'/,
     $     EOF/'!!'/
C
      OPEN(10,FILE='MACROSAVE',FORM='FORMATTED',STATUS='OLD')
C
      WRITE(2,600)
      WRITE(2,700)
      WRITE(2,800)
      WRITE(2,900)
C
C INITIALIZE MACRO COUNTER "M" & LINE COUNTER "L":
C
      M = 0
      L = 1
C
C LOOK FOR AN EXCLAMATION MARK DENOTING THE BEGINNING OF A NEW
C MACRO.
C
11    READ(10,100,END=101) CHR
      IF (ICHAR(CHR(1)).NE.33)                          GO TO 11
C
C INCREMENT THE EXTENSION # OF THE GENERIC OUTPUT JUNK FILES,
C & GENERATE THE CHARACTER VARIABLE "FILNAM".
C
21    M = M+1
      N1 = M/100 + 1
      N2 = ( M - 100*(N1-1) )/10 + 1
      N3 = M - 100*(N1-1) - 10*(N2-1) + 1
      FILNAM = CONC ( GEN, EX(N1), EX(N2), EX(N3) )
      OPEN(12,FILE= FILNAM ,FORM='FORMATTED',STATUS='NEW')
      WRITE(12,100) CHR
C
C ASSIGN AN ALPHABETIZING CODE TO THE MACRO TITLE, WITH DIGITS
C RANKED BELOW LETTERS:
C
      DO 31 I = 1, 3
            NAM(I) = ICHAR( CHR( I + 1 ) )
31          IF ( NAM(I). LT. 65 )  NAM(I) = NAM(I) + 43
            CODE(M) = 40000.*NAM(1) + 200.*NAM(2) + NAM(3)
```

```
            WRITE(2,300) CHR(2), CHR(3), CHR(4)
C
C CONTINUE READING THE FILE UNTIL THE BEGINNING OF THE NEXT
C MACRO IS ENCOUNTERED, OR 2 SUCCESSIVE EXCLAMATION MARKS ARE
C FOUND.
C
41    READ(10,100,END=101) CHR
      L = L + 1
      IF (ICHAR(CHR(1)).EQ.33) CLOSE(12)
      IF (ICHAR(CHR(1)).EQ.33.AND.ICHAR(CHR(2)).NE.33 ) GOTO 21
      IF (ICHAR(CHR(1)).EQ.33.AND.ICHAR(CHR(2)).EQ.33 ) GOTO 111
      WRITE(12,100) CHR
                                                        GOTO 41
C
C ***************************************************************
C SORT THE ALPHABETIZING CODES:
C
101   CLOSE(12)
      PRINT *,'ERROR: EOF W/O TWO EXCLAMATION MARKS '
111   CALL SORT( M, CODE, ISORT )
C
C OPEN THE OUTPUT FILE:
C
      OPEN(11, FILE = 'AMAC.NEW', FORM='FORMATTED',
     $     STATUS='UNKNOWN', SIZE=ISIZE)
C
C RETRIEVE THE MACROS IN ALPHABETICAL ORDER FROM THE "JUNK.EXT"
C FILES.  INSERT A BLANK LINE BETWEEN EACH PAIR OF SUCCESSIVE
C MACROS.  TRIM TRAILING BLANKS FROM OUTPUT.
C
            WRITE(2,400)
      DO 131 I = 1 , M
            M1 = CODE(I)/40000
            M2 = (CODE(I) - M1*40000.)/200
            M3 = CODE(I) - M1*40000. - M2*200.
            IF ( M1. GT. 90 ) M1 = M1 - 43
            IF ( M2. GT. 90 ) M2 = M2 - 43
            IF ( M3. GT. 90 ) M3 = M3 - 43
            WRITE(2,300) CHAR(M1), CHAR(M2), CHAR(M3)
            IEXT = ISORT(I)
            N1 = IEXT/100 + 1
            N2 = ( IEXT - 100*(N1-1) )/10 + 1
            N3 = IEXT - 100*(N1-1) - 10*(N2-1) + 1
            FILNAM = CONC ( GEN, EX(N1), EX(N2), EX(N3) )
            OPEN(12,FILE= FILNAM,FORM='FORMATTED',STATUS='OLD')
      DO 121 L = 1 , 1000
            READ(12,200,END=125) CHRS
121         WRITE(11,200) TRIM(CHRS,64)
125         WRITE(11,100) BLANK
131         CLOSE(12)
            WRITE(11,500) EOF
100   FORMAT(64A1)
200   FORMAT(A64)
```

```
300   FORMAT(1X,3A1)
400   FORMAT('0','ALPHABETIZED MACROS')
500   FORMAT(A2)
600   FORMAT(1X,'THIS PROGRAM ALPHABETIZES AN ASCII FILE CALLED
     $ "MACROSAVE"')
700   FORMAT(1X,'(LIBRARY OF MACROS) & SENDS THE OUTPUT TO
     $ "AMAC.NEW"')
800   FORMAT('0','************** WARNING **************')
900   FORMAT(1X,'THIS PROGRAM WILL FAIL IF THE EOF SYMBOL IN
     $ MACROSAVE IS ON THE SAME LINE AS THE !! MARKER')
      CLOSE(11)
      STOP
      END




!
C ------------------------------------------------------------
C "ASCSND.FOR"
C
C CALLS: 1)  "FTPARM.FOR"
C        2)  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: ASC
C ------------------------------------------------------------
C
      PROGRAM ASCSND
C
C THIS PROGRAM SENDS A BLOCK OF FTIR SCRATCH FILES TO ANOTHER
C COMPUTER VIA THE PRINTER PORT.  IT IS CALLED BY MACRO "ASC".
C
C THE DIMENSION 3584 CORRESPONDS TO THE # OF POINTS IN ONE
C SECTOR OF 7 COLUMNS OF SPECTRAL DATA SENT TO DISK.
C
      INTEGER IDATA(512),FSBSEC
      DIMENSION Y(3584),DSCALE(7)
C
C READ FTIR PARAMETERS:
C
      INODE  =IRVAL(13004,0)
      NSECS  =IRVAL(14001,0)
      IFILE  =IRVAL(14022,0)
      WVNI   = RVAL(14135,0)
      WVNL   = RVAL(14213,0)
      NFILES =IRVAL(14222,0)
C
C READ THE FILE STATUS BLOCKS TO GET THE HENE LASER CM-1 & THE
C FILE EXPONENTS.
C
            FSBSEC = IFILE*NSECS+88-1
      DO 11  I=1,NFILES
```

```
                CALL IRTISK(IDATA,512,FSBSEC+I*NSECS,INODE)
                IEXP   = IDATA(6)
                DSCALE(I) = 2**(19-IEXP)
                IF (I.EQ.1) THEN
                    IHENE  = IDATA(333)
                    CALL FTPARM(IHENE,WVNI,WVNL,WVNMIN,WVNMAX,
     $                              IISEC,IFSEC,INDXSP,INDXEP,PPWVN)
                    ENDIF
11              CONTINUE
C
        DO 201 M = IISEC,IFSEC
                WRDDIF = 512*(M-1)
                L = 0
                JMIN = 1
                JMAX = 512
                IF (M.EQ.IISEC) JMIN = INDXSP
                IF (M.EQ.IFSEC) JMAX = INDXEP
                NPPSEC = JMAX-JMIN+1
        DO 101 I = 1,NFILES
                MSEC=FSBSEC+(I-1)*NSECS+M
                CALL IRTISK(IDATA,512,MSEC,INODE)
        DO 31   J = JMIN,JMAX
                L = L+1
                Y(L) = IDATA(J)/DSCALE(I)
                IF (Y(L).GT.4.0)   Y(L)= 4.0
31              IF (Y(L).LT.-.99) Y(L)= -.99
101             CONTINUE
                N1 = NPPSEC
                N2 = 2*NPPSEC
                N3 = 3*NPPSEC
                N4 = 4*NPPSEC
                N5 = 5*NPPSEC
                N6 = 6*NPPSEC
                L  = 0
        DO 111 J = JMIN,JMAX
                L = L+1
                WVN = (J+WRDDIF-1)/PPWVN
                IF (NFILES.EQ.1) THEN
                      WRITE(10,300) WVN,Y(L)
                   ELSEIF (NFILES.EQ.2) THEN
                      WRITE(10,300) WVN,Y(L),Y(L+N1)
                   ELSEIF (NFILES.EQ.3) THEN
                      WRITE(10,300) WVN,Y(L),Y(L+N1),Y(L+N2)
                   ELSEIF (NFILES.EQ.4) THEN
                      WRITE(10,300) WVN,Y(L),Y(L+N1),Y(L+N2),
     $                      Y(L+N3)
                   ELSEIF (NFILES.EQ.5) THEN
                      WRITE(10,300) WVN,Y(L),Y(L+N1),Y(L+N2),
     $                      Y(L+N3),Y(L+N4)
                   ELSEIF (NFILES.EQ.6) THEN
                      WRITE(10,300) WVN,Y(L),Y(L+N1),Y(L+N2),
     $                      Y(L+N3),Y(L+N4),Y(L+N5)
                   ELSE
```

```
                WRITE(10,300) WVN,Y(L),Y(L+N1),Y(L+N2),
     $                Y(L+N3),Y(L+N4),Y(L+N5),Y(L+N6)
              ENDIF
111           CONTINUE
201           CONTINUE
              WRITE(10,400)
300           FORMAT(1X,F6.1,7(1X,F6.4))
400           FORMAT(1X,' ')
              CALL EXIT
              END




!
C ------------------------------------------------------------
C "AUTIT.FOR"
C
C CALLS: 1)  "AUTIT1.FOR"
C        2)  FTIR SYSTEM SUBROUTINES
C
C CALLING MACROS: LBB, SAM, & STI
C
C ------------------------------------------------------------
C
      PROGRAM AUTIT
C
C AUTOMATIC TITLE GENERATOR FOR FTIR FILES.
C
C          THIS PROGRAM SHOULD BE CALLED BY A SPECTRAL DATA
C COLLECTION MACRO EACH TIME A SPECTRUM IS COLLECTED, AND
C PREFERABLY BEFORE THE SPECTRUM IS DISPLAYED.  THE "SRT"
C PARAMETER IS USED TO STORE THE FILE # OF THE 1ST FILE
C IN THE BLOCK OF SPECTRA SO THAT FILE EXTENSIONS CAN BE
C ASSIGNED CORRECTLY, & THE TITLE SPECIFICATIONS CAN BE
C RETRIEVED FROM FILE SRT-1 (NOTE: TITLE SPECS CANNOT BE STORED
C IN FILES SRT OR HIGHER SINCE THE COMPUTER WRITES A NEW FSB
C EACH TIME IT COLLECTS DATA).  "DFN" IS THE CURRENT FILE TO BE
C TITLED.
C
      INTEGER IFSB(512),OFSB(512),OFILE,LDIG(4),SRTFIL
C
C READ FTIR PARAMETERS; THEN READ THE STATUS BLOCK OF THE FILE
C WHICH CONTAINS THE KEYBOARD INPUT SPECIFICATIONS FOR THE
C TITLES OF THE SPECTRAL FILES:
C
C FTIR VS. FORTRAN:
C                    SRT = SRTFIL
C                    DFN = OFILE
C
      IQUIT =  IRVAL(13736,0)
      IF (IQUIT.EQ.1)                                  GO TO 701
```

```
C
      INODE =  IRVAL(13004,0)
      NDP   =  IRVAL(14000,0)*256
      NSECS =  IRVAL(14001,0)
      OFILE =  IRVAL(14022,0)
      SRTFIL=  IRVAL(14221,0)
C
      CALL IRTISK(IFSB,512,SRTFIL*NSECS+87,INODE)
C
C READ THE OUTPUT STATUS BLOCK ARRAY WHICH HAS BEEN CREATED BY
C THE FTIR SYSTEM AFTER SPECTRAL DATA COLLECTION:
C
      CALL IRTISK(OFSB,512,(OFILE+1)*NSECS+87,INODE)
C
C INITIALIZE THE TITLE FIELD OF "OFILE" WITH BLANKS:
C
      DO 11 I=68,107
11          OFSB(I)=160
C ***************************************************************
C
C TITLE FIELD #1:  GENERIC FILE NAME
C
      NCI= 144
      NCO= 67
      CALL AUTIT1(41,NCI,NCO,IFSB,OFSB)
      IF (NCO.GE.107)                                    GO TO 601
C
C IF FIELD #1 OR #2 IS EMPTY,  SKIP TO FIELD #3.  OTHERWISE, PUT
C A PERIOD AFTER THE GENERIC FILE NAME:
C
      NCI=NCI+1
      IF (NCO.EQ.67)                                     GO TO 301
      NCO=NCO+1
      IF (IFSB(NCI).EQ.170)                              GO TO 221
      IF (NCO.LE.107) OFSB(NCO)=174
C
C ***************************************************************
C
C TITLE FIELD #2:  FILE EXTENSION #
C
            NDIG=0
      DO 201 I=1,4
            IF (IFSB(NCI).EQ.170)                        GO TO 211
            NCI=NCI+1
201         NDIG=NDIG+1
            PRINT *,'ERROR: NO * AFTER TITLE EXTENSION FIELD'
                                                         GO TO 601
211                     IEXT=OFILE-SRTFIL + IFSB(NCI-1)-176
            IF (NDIG.GT.1) IEXT=IEXT+ 10*(IFSB(NCI-2)-176)
            IF (NDIG.GT.2) IEXT=IEXT+100*(IFSB(NCI-3)-176)
            IDIG=IEXT/100
            OFSB(NCO+1)=IDIG+176
            IREM=IEXT-100*IDIG
```

```
            IDIG=IREM/10
            OFSB(NCO+2)=IDIG+176
            OFSB(NCO+3)=IREM-10*IDIG+176
C
C PUT A BLANK AFTER THE FILE EXTENSION #:
C
      NCO=NCO+4
221   IF (NCO.LE.107) OFSB(NCO)=160
C
C ****************************************************************
C
C TITLE FIELD #3:  DESCRIPTOR
C
C EXAMINE THE 1ST CHARACTER OF THE DESCRIPTOR. IF IT IS AN
C ASTERISK, SKIP TO THE NEXT FIELD; IF IT IS A BLANK, IGNORE IT
C SINCE A BLANK HAS ALREADY BEEN PLACED AFTER THE FILE
C EXTENSION #.  IF IT IS NOT A BLANK, SEND IT TO THE OUTPUT FSB
C ARRAY.
C
301   NCI=NCI+1
      IF (IFSB(NCI).EQ.170)                                GO TO 401
      IF (IFSB(NCI).EQ.160)                                GO TO 311
      NCO=NCO+1
      IF (NCO.LE.107) OFSB(NCO)= IFSB(NCI)
311   CALL AUTIT1(41,NCI,NCO,IFSB,OFSB)
C
C IF THE LAST LETTER OF THE DESCRIPTOR WAS A BLANK, SKIP TO
C FIELD #4.  IF IT WASN'T, INSERT A BLANK INTO THE OUTPUT ARRAY.
C
      IF (IFSB(NCI-1).EQ.160)                              GO TO 401
      NCO=NCO+1
      OFSB(NCO)=160
C
C ****************************************************************
C TITLE FIELD #4:  ELAPSED TIME
C
C DETERMINE WHETHER THE MONTH OF THE CURRENT SPECTRUM AGREES
C WITH THE MONTH OF THE T=0 TIME.  ASSUME THAT THE MONTH HAS
C NOT CHANGED BY MORE THAN 1 UNIT:
C
401   NCI = NCI + 1
      IF (IFSB(NCI).EQ.170)                                GO TO 501
      MONDIF= OFSB(50) - IFSB(NCI+1)
      INCDAY=0
      IF (MONDIF.EQ.0)                                     GO TO 411
C
C COMPUTE TIME DIFFERENCES DIRECTLY FROM ASCII INTEGER CODES.
C COMPUTE ABSOLUTE TIMES BY SUBTRACTING 176 FROM ASCII CODES.
C
      MO= 10*(IFSB(NCI)-176) + IFSB(NCI+1) - 176
                                                           INCDAY=31
      IF (MO.EQ.4.OR.MO.EQ.6.OR.MO.EQ.9.OR.MO.EQ.11)       INCDAY=30
      IF (MO.EQ.2)                                         INCDAY=28
```

```
411    DAYDIF= 10 * (OFSB(52)-IFSB(NCI+2))
       DAYDIF= DAYDIF+ OFSB(53) - IFSB(NCI+3) + INCDAY
       HRDIF = 10 * (OFSB(58)-IFSB(NCI+4))
       HRDIF = HRDIF + OFSB(59) - IFSB(NCI+5) + DAYDIF*24
       FHRDIF= 10 * (OFSB(61)-IFSB(NCI+6))
       FHRDIF= (FHRDIF + OFSB(62) - IFSB(NCI+7) ) / 60
       HRDIF = HRDIF + FHRDIF
C
C DETERMINE EACH DIGIT OF THE ELAPSED TIME, CONVERT EACH BACK TO
C ASCII CODE, AND SEND CODES TO THE OUTPUT FSB:
C
       IF (HRDIF.LT.0.0) PRINT *,'ERROR: NEGATIVE ELAPSED TIME'
       IF (HRDIF.LT.0.0)                                    GO TO 601
             NCO       = NCO + 1
421          N         = ALOG10(HRDIF)
             OFSB(NCO) = 176
             REM       = HRDIF
       DO 431 I = 1, 4
             J = I - 1
             IF (I. GT. N+1)                                GO TO 441
             Q           = 10**(N-J)
             LDIG(I)     = INT( 0.001 + REM/Q )
             REM         = REM - Q*LDIG(I)
431          OFSB(NCO+J) = LDIG(I) + 176
441          IF (N.LT.0) J=1
C
C SEND ".# HR" TO THE OUTPUT ARRAY:
C
             OFSB(NCO+J)   = 174
             NR            = NINT(10*REM)
             IF (NR. EQ. 10) HRDIF = HRDIF + 0.05
             IF (NR. EQ. 10)                                GO TO 421
             OFSB(NCO+J+1) = NR + 176
             OFSB(NCO+J+2) = 160
             OFSB(NCO+J+3) = 200
             OFSB(NCO+J+4) = 210
             OFSB(NCO+J+5) = 160
             NCO           = NCO + J + 5
             NCI           = NCI + 8
C
C ***************************************************************
C TITLE FIELD #5: DATE
C
501          NCI = NCI + 1
C
C OMIT THE DATE IF NO "D" APPEARS IN INPUT TITLE SPECIFICATION
C FIELD #5 OR IF THERE IS NOT ENOUGH SPACE LEFT IN THE OUTPUT
C TITLE FIELD:
C
             IF (IFSB(NCI).NE.196)                          GO TO 601
             IF (NCO.GT.100)                                GO TO 601
             CALL AUTIT1(8,48,NCO,OFSB,OFSB)
601          CALL IWTISK(OFSB,512,(OFILE+1)*NSECS+87,INODE)
```

```
701    CALL EXIT
       END



!
C ------------------------------------------------------------
C "AUTIT1.FOR"
C
C SUBROUTINE OF "AUTIT.FOR"
C ------------------------------------------------------------
C
       SUBROUTINE AUTIT1(IMAX,NCI,NCO,IFSB,OFSB)
C
       INTEGER IFSB(512),OFSB(512)
C
C DIRECTLY TRANSFER THE CHARACTERS OF THE INPUT TITLE FIELD TO
C THE OUTPUT TITLE FIELD UNTIL AN ASTERISK (ASCII CODE 170) IS
C ENCOUNTERED OR "IMAX" CHARACTERS HAVE BEEN TRANSFERRED.
C
       DO 101  I=1,IMAX
               NCI=NCI+1
               IF (IFSB(NCI).EQ.170)                    GO TO 201
               NCO=NCO+1
101            IF (NCO.LE.107) OFSB(NCO)=IFSB(NCI)
201            RETURN
               END



!
C ------------------------------------------------------------
C "AXIS2.FOR"
C
C SUBROUTINE OF "PLOTFT.FOR"
C
C ------------------------------------------------------------
C
       SUBROUTINE AXIS2 (USTART,   UEND,   XPN0,   YPN0, AXSPAN,
      1                  AXANGL, SZMJTC, TICRAT, TSZRAT, BEGNUM,
      2                  SPCNUM, DECDIG, SIZNUM, DSTNUM, JSTNUM,
      3                  ANGNUM, LETTRS, NLET  , SIZLET, DSTLET,
      4                  CNTLET,ANGLET)
C
       INTEGER TICRAT,TR1,DECDIG,AXFLIP,SGNAXS,LETTRS(88)
       REAL NUMJST,JSTNUM
C
C ************************************************************
C A NEGATIVE "SIZNUM" KILLS TICS & TIC LABELS.
```

```
C "    "     "SIZLET"    "   AXIS LABEL.
C
      IF (DECDIG.LE.0) DECDIG=-1
      SPANMX=0.0
      IAXROT=0
      NUMROT=0
      LETROT=0
      AXFLIP=0
      NUMFLP=0
      LETFLP=0
      SGNAXS=1
      NSTEPS=0
      ILABEL=0
      SPACNM=SPCNUM
      DISLET=DSTLET
      NUMJST=SIZNUM*JSTNUM
      IF (NINT(AXANGL).EQ.90.OR.NINT(AXANGL).EQ.270) IAXROT=1
      IF (NINT(AXANGL).EQ.180.OR.NINT(AXANGL).EQ.270) AXFLIP=1
      IF (NINT(ANGNUM).EQ.90.OR.NINT(ANGNUM).EQ.270) NUMROT=1
      IF (NINT(ANGNUM).EQ.180.OR.NINT(ANGNUM).EQ.270) NUMFLP=1
      IF (NINT(ANGLET).EQ.90.OR.NINT(ANGLET).EQ.270) LETROT=1
      IF (NINT(ANGLET).EQ.180.OR.NINT(ANGLET).EQ.270) LETFLP=1
      S1=2*AXFLIP-1
      S2=2*NUMFLP-1
      S3=NUMFLP-AXFLIP
      S4=1-AXFLIP-NUMFLP
      S5=2*LETFLP-1
      S6=LETFLP-AXFLIP
      S7=1-AXFLIP-LETFLP
C
C ***************************************************************
C ************************ DRAW AXIS ****************************
C
      IF (AXSPAN.LT.0) SGNAXS=-1
C
C INITIALIZE PLOTTER AND THEN MOVE PEN TO AXIS ORIGIN.
C
      CALL PLOT(XPN0,YPN0,3)
C
C LOCATE END OF AXIS; THEN DRAW AND RETRACE THE AXIS.
C
      XPN=XPN0+(1-IAXROT)*AXSPAN
      YPN=YPN0+IAXROT*AXSPAN
      CALL PLOT(XPN,YPN,2)
      CALL PLOT(XPN0,YPN0,2)
      IF (SIZNUM.LE.0.0)                                  GO TO 121
C
C DETERMINE TIC LOCATION IN INCHES (TICLOC) FOR FIRST TIC:
C
            IF (UEND.LT.USTART.AND.SPACNM.GT.0.0) SPACNM=-SPACNM
              UPINCH=(UEND-USTART)/ABS(AXSPAN)
              TICLOC=(BEGNUM-USTART)/UPINCH
              SPMJTC=SPACNM/UPINCH
```

```
            TR1=TICRAT+1
            SPMINR=SPMJTC/TR1
         DO 61 I=1,TICRAT+1
            TICLOC=TICLOC-SPMINR
            IF (TICLOC.LE.-0.01)                          GO TO 81
            NSTEPS=NSTEPS+1
61          CONTINUE
81          TICLOC=TICLOC+SPMINR
C
C COMPUTE THE TOTAL NUMBER OF TICS.  A '1.01' VALUE IS USED IN
C PLACE OF '1.00' TO AVOID TRUNCATION ERRORS IN CONVERTING FROM
C A REAL NUMBER TO AN INTEGER.
C
            NTICS=1.01+(ABS(AXSPAN)-TICLOC)/SPMINR
C
C ****************************************************************
C ************* DRAW AND LABEL THE TIC MARKS *********************
C
               ICOUNT=0
          DO 111 I=0,NTICS-1
C
C DETERMINE WHETHER THE UPCOMING TIC IS MAJOR OR MINOR:
C
               ILARGE=0
               NQ=I-NSTEPS
               IF (TR1*(NQ/TR1).EQ.NQ) ILARGE=1
               TICSIZ=ILARGE*SZMJTC+(1-ILARGE)*SZMJTC/TSZRAT
C
C LOCATE THE POSITION OF THE UPCOMING TIC AND THEN MOVE THE
C PEN THERE.
C
               TICNXT=TICLOC+I*SPMINR
               XPN=XPN0+(1-IAXROT)*SGNAXS*TICNXT
               YPN=YPN0+IAXROT*SGNAXS*TICNXT
               CALL PLOT(XPN,YPN,2)
C
C DETERMINE THE COORDINATES OF THE END OF THE TIC MARK AND
C THEN MOVE THE PEN THERE.
C
               XPN2=XPN
               YPN2=YPN
               IF (IAXROT.EQ.1) XPN2=XPN2-S1*TICSIZ
               IF (IAXROT.EQ.0) YPN2=YPN2+S1*TICSIZ
               CALL PLOT(XPN2,YPN2,2)
               IF (ILARGE.NE.1)                           GO TO 111
C
C IF TIC IS MINOR, SKIP TO END OF TIC LOOP; IF TIC IS MAJOR,
C DETERMINE HOW MANY CHARACTERS ARE PRESENT IN THE NUMBER LABEL
C (INCLUDING THE DECIMAL POINT, IF PRESENT).  THIS VALUE IS
C NEEDED FOR DETERMINING WHERE TO POSITION THE PEN FOR THE
C 'NUMBER' SUBROUTINE.
C     'NNUM' IS INITIALLY SET AT THE MINIMUM TOTAL DIGITS
C POSSIBLE FOR THE GIVEN # OF DIGITS TO THE RIGHT OF THE DECIMAL
```

```
C PT.  IT IS LATER INCREMENTED BY 'MORDIG' IF THE LOGARITHM OF
C THE # LABEL SHOWS THAT MORE DIGITS ARE REQUIRED.
C
               NNUM=2+DECDIG
               IF (DECDIG.EQ.0) NNUM=1
               RNUM=BEGNUM+ILABEL*SPACNM
               IF (RNUM.LT.0)   NNUM=NNUM+1
               NROUND=NINT(RNUM)
               ILABEL=ILABEL+1
               IF (NROUND.LT.10)                          GO TO 101
C
C THE '0.0001' TERM BELOW IS USED TO PREVENT TRUNCATION ERRORS.
C
               MORDIG=INT(ALOG10(0.0001+NROUND))
               NNUM=NNUM+MORDIG
C
C 'SPANUM' IS THE LENGTH OF THE CURRENT # LABEL IN INCHES.
C 'SPANMX' IS THE LENGTH OF THE LONGEST # LABEL, AND IS LATER
C USED FOR CALCULATING WHERE TO POSITION THE AXIS NAME.
C
101            SPANUM=(NNUM-0.5)*SIZNUM
               IF (SPANUM.GE.SPANMX) SPANMX=SPANUM
C
C THE FOLLOWING STEPS ARE USED TO LOCATE THE (X,Y) COORDINATES
C OF THE FIRST CHARACTER OF EACH OF THE NUMBER LABELS (XPNUMB
C & YPNUMB).  THIS CALCULATION IS BASED ON THE INPUT PARAMETERS
C 'DSTNUM', 'SIZNUM' AND 'JSTNUM'; AND IT TAKES ACCOUNT OF THE
C VARIOUS NUMBER AND AXIS ORIENTATIONS THAT MAY BE REQUESTED.
C COORDINATES THAT DEPEND ON THE # OF DIGITS IN THE # LABEL MUST
C BE CALCULATED FOR EACH TIC LOOP ITERATION SINCE THE # OF
C DIGITS MAY VARY.
C
       IF (ICOUNT.GT.0)                                   GO TO 105
       ICOUNT=ICOUNT+1
       IF (IAXROT.EQ.0.AND.NUMROT.EQ.1) XN=-S2*0.5*SIZNUM
       IF (IAXROT.EQ.1.AND.NUMROT.EQ.1) XN=-S1*DSTNUM+S4*SIZNUM
       IF (IAXROT.EQ.0.AND.NUMROT.EQ.0) YN=S1*DSTNUM-S4*SIZNUM
       IF (IAXROT.EQ.1.AND.NUMROT.EQ.0) YN=S2*0.5*SIZNUM
105    IF (IAXROT.EQ.0.AND.NUMROT.EQ.0) XN=S2*(SPANUM-NUMJST)
      IF (IAXROT.EQ.1.AND.NUMROT.EQ.0) XN=-S1*DSTNUM+S3*SPANUM
      IF (IAXROT.EQ.0.AND.NUMROT.EQ.1) YN=S1*DSTNUM-S4*SPANUM
      IF (IAXROT.EQ.1.AND.NUMROT.EQ.1) YN=S2*(SPANUM-NUMJST)
        XPNUMB=XPN2+XN
        YPNUMB=YPN2+YN
C
C LIFT THE PEN AND MOVE IT TO THE LOWER LEFT CORNER OF THE
C FIRST DIGIT OF THE NUMBER LABEL.  THEN, DRAW THE NUMBER,
C RETURN TO THE BOTTOM OF THE TIC MARK, PUT THE PEN DOWN, AND
C RETRACE THE TIC MARK.
C
       CALL PLOT(XPNUMB,YPNUMB,3)
       CALL NUMBER(XPNUMB,YPNUMB,SIZNUM,RNUM,ANGNUM,DECDIG)
       CALL PLOT(XPN2,YPN2,3)
```

```
111     CALL PLOT(XPN,YPN,2)
C
C RETURN PEN TO AXIS ORIGIN WITH PEN DOWN.
C
        CALL PLOT(XPN0,YPN0,2)
C
C ********************************************************************
C ****************** DRAW THE AXIS NAME ******************************
C
C USE THE PARAMETERS 'DISLET', 'SIZLET', AND 'NLET' TO DETERMINE
C THE COORDINATES OF THE LOWER LEFT CORNER OF THE 1ST CHARACTER
C OF THE AXIS NAME.  THIS CALCULATION TAKES ACCOUNT OF THE
C VARIOUS LETTER AND AXIS ORIENTATIONS THAT MAY BE REQUESTED.
C
      IF (IAXROT.EQ.NUMROT) BNDRY=ABS(S3)*SIZNUM
      IF (IAXROT.EQ.1.AND.NUMROT.EQ.0) BNDRY=ABS(S4)*SPANMX
      IF (IAXROT.EQ.0.AND.NUMROT.EQ.1) BNDRY=ABS(S3)*SPANMX
      DISLET=DISLET+BNDRY+IAXROT*ABS(XPN0-XPNUMB)
      DISLET=DISLET+(1-IAXROT)*ABS(YPN0-YPNUMB)
121   IF (SIZLET.LE.0.0.OR.NLET.LE.0)                    GO TO 199
      SPANLT=(NLET-0.5)*SIZLET
      IF (IAXROT.EQ.0.AND.LETROT.EQ.0) XPN=S5*0.5*SPANLT
      IF (IAXROT.EQ.0.AND.LETROT.EQ.1) XPN=-S5*0.5*SIZLET
      IF (IAXROT.EQ.1.AND.LETROT.EQ.0) XPN=-S1*DISLET+S6*SPANLT
      IF (IAXROT.EQ.1.AND.LETROT.EQ.1) XPN=-S1*DISLET+S7*SIZLET
      IF (IAXROT.EQ.0.AND.LETROT.EQ.0) YPN=S1*DISLET-S7*SIZLET
      IF (IAXROT.EQ.0.AND.LETROT.EQ.1) YPN=S1*DISLET-S7*SPANLT
      IF (IAXROT.EQ.1.AND.LETROT.EQ.0) YPN=S5*0.5*SIZLET
      IF (IAXROT.EQ.1.AND.LETROT.EQ.1) YPN=S5*0.5*SPANLT
      XPN=XPN+XPN0+(1-IAXROT)*(0.5*AXSPAN+CNTLET)
      YPN=YPN+YPN0+IAXROT*(0.5*AXSPAN+CNTLET)
       CALL SYMBOL(XPN,YPN,-SIZLET,LFTTRS,ANGLET,NLET)
199    CALL PLOT(0,0,3)
      RETURN
      END




!
C ------------------------------------------------------------------
C "BASLIN.FOR"
C
C CALLS: 1)  "FTPARM.FOR"
C        2)  "SPLINE.FOR" > "MATINV.FOR"
C        3)  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: BSL
C
C ------------------------------------------------  ------------
C
      PROGRAM BASLIN
```

```
C
C THIS PROGRAM IS INTENDED PRIMARILY FOR REMOVING FRINGES FROM
C MATRIX-ISOLATION SPECTRA.  BASELINE PTS ARE SENT TO FILE 0
C & NICOS FILE "BASLIN.DAT".  POORLY CHOSEN BASELINE PTS CAN BE
C DELETED FROM "BASLIN.DAT" USING TED.  RERUNNING "BSL" USING
C THE VI1=0 OPTION WILL GENERATE A REVISED BASELINE-CORRECTED
C SPECTRUM.  CM-1 RANGES CONTAINING BROAD PEAKS SHOULD BE
C SKIPPED AS THEY WILL OTHERWISE PRODUCE BAD BASELINE REF PTS.
C
      INTEGER   DRDATA(512),OZDATA(512),NICSEC(4),NICWRD(4),
     1          FSKIP(3,2),IBSKIP(3,2),LIMWRD(3,2),
     2          BASCNT,BSLINE,BLKSIZ,ENDATA,OZFN,OZFSEC,BSFIND,
     3          ODFSEC,ODFN,OLDSEC,ZSCALE
      INTEGER*2 ISIZE
      DIMENSION BFRQ(10),YD(10),CD(10,3)
C
      DATA NBLANK/0/ ,LASTPT/0/  ,ICNT  /0/  ,ICD   /0/ ,
     1     BASCNT/0/ ,ENDATA/512/,IH    /4/ ,
     2     OLDSEC/0/ ,ISTART/1/
C
C ****************************************************************
C
      OPEN(11,FILE='BASLIN.DAT', FORM='FORMATTED',
     $        STATUS='UNKNOWN', SIZE=ISIZE)
C
C ****************************************************************
C ****************** FTIR PARAMETERS *************************
C
      BSFIND     = IRVAL(13763,0)
      IRFN       = IRVAL(14030,0)
      ODFN       = IRVAL(14022,0)
      OZFN       = IRVAL(14023,0)
      RFXF       =  RVAL(14135,0)
      RLXF       =  RVAL(14213,0)
      NSECS      = IRVAL(14001,0)
      INODE      = IRVAL(13004,0)
      FSKIP(1,1) = IRVAL(13732,0)
      FSKIP(1,2) = IRVAL(13715,0)
      FSKIP(2,1) = IRVAL(13736,0)
      FSKIP(2,2) = IRVAL(14177,0)
      FSKIP(3,1) = IRVAL(14012,0)
      FSKIP(3,2) = IRVAL(13760,0)
C
C COMPUTE SECTOR INDICES FOR USE IN IRTISK AND IWTISK ROUTINES:
C
      IRFSEC=IRFN*NSECS+88-1
      ODFSEC=ODFN*NSECS+88-1
      OZFSEC=OZFN*NSECS+88-1
C
C READ FILE STATUS BLOCK TO GET HE-NE LASER CM-1:
C
      CALL IRTISK(DRDATA,512,IRFSEC+NSECS,INODE)
      IHENE=DRDATA(333)
```

```
C
C ****************************************************************
C COMPUTE SPECTRAL RANGE PARAMETERS WITH "FTPARM.FOR"
C
      CALL FTPARM(IHENE,RFXF,RLXF,FRQMIN,FRQMAX,IISEC,IFSEC,
     1            INDXSP,INDXEP,PPWVN)
C
            NX=-524288
            ZSCALE=-NX/4
            IF (BSFIND.EQ.0)                              GO TO 261
            WRITE (2,8000)
            BLKSIZ = IRVAL(13762,0)
            BLKSIZ=16*(BLKSIZ/16)
            IF (BLKSIZ.LT.16) BLKSIZ=16
            NBLKS=512/BLKSIZ
C ****************************************************************
C COMPUTE ARRAY INDICES CORRESPONDING TO THE CM-1 LIMITS OF
C RANGES TO BE SKIPPED BY THE BASELINE-LOCATOR ALGORITHM:
C
      DO 31  I = 1, 3
            IF ( FSKIP(I,1). GT. FSKIP(I,2) ) THEN
                 TMP         = FSKIP(I,2)
                 FSKIP(I,2) = FSKIP(I,1)
                 FSKIP(I,1) = TMP
                 ENDIF
31          CONTINUE
      DO 51  I = 1, 2
      DO 41  J = 1, 3
            IX           = PPWVN * FSKIP(J,I)
            IBSKIP(J,I) = IX / BLKSIZ + 1
41          LIMWRD(J,I) = IX - ( (IX-1)/512 ) * 512
51          CONTINUE
C
C****************************************************************
C ***************** LOCATE BASELINE POINTS **********************
C
      DO 251 M = IISEC, IFSEC
            IIBLK  = 1
            WRDDIF = 512 * (M-1)
            CALL IRTISK( DRDATA, 512, IRFSEC+M, INODE)
            IF ( M. NE. IISEC )                           GO TO 191
C
C ****************************************************************
C FIRST SECTOR ONLY:
C
            IIBLK  = INDXSP / BLKSIZ + 1
            FRQMIN = ( WRDDIF + INDXSP - 1 ) / PPWVN
            WRITE(11,8300) BLKSIZ
            WRITE(11,8500) FRQMIN, RFXF, RLXF
C
C ****************************************************************
C THE CURRENT SPECTRAL DATA BLOCK IS EXAMINED TO FIND THE
C MINIMUM ABSORBANCE.
```

```
C
191    DO 241  LOCBLK = IIBLK, NBLKS
               IBLK   = ( M-1 ) * NBLKS + LOCBLK
              IF ( M. EQ. IFSEC. AND. LOCBLK*BLKSIZ. GE. INDXEP)
     1           LASTPT = INDXEP
              ILAST  = LOCBLK * BLKSIZ
              IFIRST = ILAST - BLKSIZ + 1
              IF (BASCNT.EQ.0) IFIRST = INDXSP
              IF (LASTPT.NE.0) ILAST  = INDXEP
       DO 195 I = 1, 3
              IF (IBLK.GT.IBSKIP(I,1).AND.IBLK.LT.IBSKIP(I,2))
     1                                                  GO TO 241
              IF ( IBLK. EQ. IBSKIP(I,1) ) ILAST  = LIMWRD(I,1)
195           IF ( IBLK. EQ. IBSKIP(I,2) ) IFIRST = LIMWRD(I,2)
              IBSWRD = IFIRST
       DO 201 I = IFIRST, ILAST
              IF ( DRDATA(IBSWRD). EQ. NX ) IBSWRD = I
              IF ( DRDATA(I). EQ. NX )                    GO TO 201
              IF ( DRDATA(I). LT. DRDATA(IBSWRD) ) IBSWRD = I
201           CONTINUE
C
C ****************************************************************
C     THE CM-1 OF EACH BASELINE PT IS SENT TO FILE "BASLIN.DAT"
C ALONG WITH THE ABSORBANCE AT THIS CM-1.
C
              WVN = ( IBSWRD + WRDDIF - 1 ) / PPWVN
              BASCNT = BASCNT + 1
              WRITE(11,8400) WVN, DRDATA(IBSWRD), M, IBSWRD
              IF ( LASTPT. EQ. 0 )                        GO TO 241
              FRQMAX = - ( WRDDIF + INDXEP - 1 ) / PPWVN
              WRITE(11,8400) FRQMAX
                                                          GO TO 251
241           CONTINUE
251           CONTINUE
              CLOSE(11)
C ****************************************************************
C ****************************************************************
C    THE SET OF BASELINE FREQUENCIES AND INTENSITIES PREVIOUSLY
C SENT TO FILE "BASLIN.DAT" ARE READ FROM THIS FILE, AND
C CUBIC SPLINE FITS ARE DONE ON SETS OF 4 CONSECUTIVE BASELINE
C PTS.  THE COEFFICIENTS DESCRIBING THE RANGE FROM PTS 2 TO 3
C ARE USED FOR BASELINE INTERPOLATION.  THEN, ARRAY INDICES 2-4
C ARE REINDEXED AS 1-3, A SEARCH IS MADE FOR THE NEXT BASELINE
C PT #4, AND ANOTHER CUBIC FIT IS PERFORMED, ETC.  FOR THE
C INITIAL AND FINAL SETS OF PTS, ADDITIONAL INTERPOLATIONS ARE
C DONE OUTSIDE OF THE USUAL 2-3 RANGE.
C
261           WRITE(2,6700)
C
C MAKE SURE THAT THE EXPONENT OF THE BASELINE DISPLAY FILE IS
C SET TO A REASONABLE VALUE:
C
              CALL IRTISK( OZDATA, 512, OZFSEC + NSECS, INODE )
```

```
              OZDATA(6) = 2
              CALL IWTISK( OZDATA, 512, OZFSEC + NSECS, INODE )
C
              M      = IISEC
              BASCNT = 2
              CALL IRTISK( DRDATA, 512, IRFSEC + IISEC, INODE )
              READ( 11, 8300 ) BLKSIZ
              READ( 11, 8500 ) FRQMIN
              INDXSP = NINT( FRQMIN * PPWVN + 1 - (IISEC-1)*512 )
              IMIN   = INDXSP
        DO 271 I = 1, 4
              READ( 11, 8400) BFRQ(I), JD, NICSEC(I), NICWRD(I)
271           YD(I)  = JD
              WRDHI  = NINT( BFRQ(1)*PPWVN + 1 - (IISEC-1)*512 )
              WRDLOW = WRDHI
281           IMAX   = 512
              IF ( IMAX. GT. WRDHI) IMAX = WRDHI
C
C FOR THE CM-1 RANGE PRECEDING THE 1ST BASELINE PT, THE
C ABSORBANCE OF THE 1ST BASELINE PT IS SUBTRACTED FROM EACH RAW
C ABSORBANCE VALUE (I.E. CUBIC SPLINES ARE NOT USED).
C
        DO 291 I = IMIN, IMAX
              IF ( DRDATA(I). EQ. NX )                    GO TO 291
              DRDATA(I) = DRDATA(I) - YD(1)
291           CONTINUE
              IF ( IMAX. EQ. 512 )                        GO TO 451
C
C ***************************************************************
C THE MAIN BASELINE CORRECTION ALGORITHM BEGINS HERE WHENEVER
C THE MOST RECENTLY READ BASELINE PT DOES NOT LIE IN A NEW
C SECTOR OF THE FTIR SCRATCH FILE.
C
301           IMIN = IMAX + 1
311           IF (IQUIT-1)                          321,315,451
C
C CHANGE THE REF PT OF THE FINAL CUBIC EQN FROM PT 3 TO PT 4 FOR
C EXTRAPOLATION OF THE CUBIC FIT BEYOND THE FINAL BASELINE PT.
C
315           D       = BFRQ(4) - BFRQ(3)
              CD(3,1) = 3* CD(3,3) *D*D + 2* CD(3,2) *D + CD(3,1)
              CD(3,2) = 0.0
              IQUIT   = IQUIT + 1
C
321           BASCNT  = BASCNT + 1
              IF ( BASCNT. EQ. 4. OR. IQUIT. NE. 0 )   GO TO 421
              IF ( BASCNT. EQ. 3 )                     GO TO 411
C
C FOR EACH BASELINE PT, DRAW A SPIKE IN THE BASELINE DISPLAY
C FILE.
C
              KMIN = 4
              IF ( BASCNT. EQ. 5)  KMIN = 1
```

```
      DO 381 K   = KMIN, 4
             NSK = NICSEC(K)
             NWK = NICWRD(K)
             IF ( NSK. NE. OLDSEC. AND. OLDSEC. NE. 0 )
     1           CALL IWTISK( OZDATA, 512, OZFSEC+OLDSEC, INODE)
             IF ( NSK. NE. OLDSEC )
     1           CALL IRTISK( OZDATA, 512, OZFSEC+NSK, INODE )
             OLDSEC      = NSK
             OZDATA(NWK) = ZSCALE
      DO 351 L = 1, IH
             IF (NWK.GT.L)       OZDATA(NWK-L) = ZSCALE*(1+.1*L)
351          IF (NWK+L.LE.512)   OZDATA(NWK+L) = ZSCALE*(1+.1*L)
C
C THE FOLLOWING STEPS DEAL WITH SPIKES IN THE BASELINE DISPLAY
C FILE THAT STRADDLE A SECTOR BOUNDARY:
C
             IF ( NWK+IH. GT. 512. AND. NSK. NE. IFSEC) THEN
                 CALL IWTISK( OZDATA, 512, OZFSEC+NSK,   INODE )
                 CALL IRTISK( OZDATA, 512, OZFSEC+NSK+1, INODE)
                 OLDSEC = NSK + 1
                 LMAX   = NWK - 512 + IH
      DO 361     L = 1, LMAX
361              OZDATA(L) = ZSCALE* ( 1 + .1*(IH + L - LMAX) )
                 ENDIF
             IF ( NWK. LE. IH. AND. NSK. NE. IISEC ) THEN
                 CALL IWTISK( OZDATA, 512, OZFSEC + NSK, INODE)
                 CALL IRTISK( OZDATA, 512, OZFSEC + NSK-1,INODE)
                 OLDSEC = NSK - 1
                 LMAX   = IH + 1 - NWK
      DO 371     L = 1, LMAX
371              OZDATA(513-L) = ZSCALE* ( 1 + .1*(IH + L-LMAX))
                 ENDIF
381          CONTINUE
                 CALL IWTISK( OZDATA, 512, OZFSEC+OLDSEC, INODE)
C
C THE (I+1)TH BASELINE INDEX FOR THE OLD BASELINE ARRAYS
C BECOMES THE ITH BASELINE INDEX FOR THE NEW ARRAYS.
C
      DO 401 I = 1, 3
             BFRQ(I) = BFRQ(I+1)
401            YD(I) =  YD(I+1)
             READ(11,8400) BFRQ(4), JD, NICSEC(4), NICWRD(4)
             YD(4) = JD
             IF ( BFRQ(4). LT. 0.0 ) THEN
                 IQUIT   = 1
                 BFRQ(4) = -BFRQ(4)
                 ENDIF
411          IF ( IQUIT. EQ. 0 ) THEN
                CALL SPLINE( 1, 4, BFRQ, YD, 0.0, 0.0, CD)
                ENDIF
C
C "J" INDICATES WHICH CM-1 VALUE IS THE REFERENCE FOR THE KTH
C SET OF SPLINE COEFFICIENTS.  K DIFFERS FROM J ON THE LAST
```

```
C INTERPOLATION BECAUSE "BFRQ" IS REINDEXED BUT THE "CD" COEFFS
C ARE NOT.
C
421           J = 2 + ( IQUIT / 2 ) - ISTART
              K = 2 + ( IQUIT + 1 ) / 2 - ISTART
              ISTART = 0
              WRDLOW = WRDHI
              WRDHI  = NINT( BFRQ(J+1) * PPWVN + 1 - (M-1)*512 )
C
C RESUME AT LINE 431 AFTER A NEW SECTOR HAS BEEN READ (I.E WHEN
C INTERPOLATION CORRECTIONS HAVE BEEN INTERRUPTED BY A SECTOR
C BOUNDARY).
C
431           IMAX = 512
              IF ( IMAX. GT. WRDHI ) IMAX = WRDHI
      DO 441  I = IMIN, IMAX
              IF ( DRDATA(I). EQ. NX )                    GO TO 441
              XD = ( I - WRDLOW ) / PPWVN
              DBASE=YD(J)+CD(K,1)*XD+CD(K,2)*XD*XD+CD(K,3)*XD**3
              DRDATA(I) = DRDATA(I) - DBASE
441           CONTINUE
              IF ( IMAX. NE. 512 )                        GO TO 301
451           CALL IWTISK( DRDATA, 512, ODFSEC + M, INODE )
              M = M + 1
              IF ( M. GT. IFSEC )                       GO TO 1999
              CALL IRTISK( DRDATA, 512, IRFSEC + M, INODE )
              IMIN = 1
              WRDLOW = WRDLOW - 512
              WRDHI  = WRDHI  - 512
              IF ( WRDHI. EQ. 0 )                         GO TO 311
C
C GO TO LINE 281 ONLY IF THE 1ST BASELINE PT OF THE SPECTRUM
C HAS NOT BEEN REACHED YET.  SUCH A SITUATION OCCURS ONLY IF THE
C 1ST BASELINE PT DOES NOT LIE IN THE 1ST SECTOR.
C
              IF (ISTART)                             1999,431,281
6700           FORMAT('0','BEGIN BASELINE CORRECTIONS')
8000           FORMAT('0','BEGIN BASELINE-LOCATOR ALGORITHM')
8300           FORMAT(I10)
8400           FORMAT(F10.3,3I10)
8500           FORMAT(3F10.3)
1999           CALL EXIT
               END



!
C ---------------------------------------------------------------
C "BLANKX.FOR"
C
C CALLS: 1)   "FTPARM.FOR"
C        2)   FTIR SYSTEM SUBROUTINES
C
```

```
C CALLING MACRO: BLX
C
C ---------------------------------------------------------------
C
      PROGRAM BLANKX
C
      DIMENSION IDATA(512)
C
C READ FTIR PARAMETERS:
C
              NSECS =IRVAL(14001,0)
              INODE =IRVAL(13004,0)
              WVNB  =IRVAL(14025,0)
              WVNE  =IRVAL(14026,0)
              IDFN  =IRVAL(14022,0)
C
              NX    =-524288
              IDFSEC=IDFN*NSECS+88-1
C
C READ THE HE-NE CM-1 FROM THE FSB OF FTIR SCRATCH FILE 0, AND
C THEN SET BOUNDARY PARAMETERS:
C
              CALL IRTISK(IDATA,512,ISEC+NSECS,INODE)
              IHENE =IDATA(333)
      CALL FTPARM(IHENE,WVNB,WVNE,FRQMIN,FRQMAX,IISEC,IFSEC,
     1            INDXSP,INDXEP,PPWVN)
C
C EXECUTE BLANKING ALGORITHM:
C
      DO 201 M=IISEC,IFSEC
              IWORD=1
              LWORD=512
              IF (M.EQ.IISEC) IWORD=INDXSP
              IF (M.EQ.IFSEC) LWORD=INDXEP
              CALL IRTISK(IDATA,512,IDFSEC+M,INODE)
      DO 101 I=IWORD,LWORD
101           IDATA(I)=NX
201           CALL IWTISK(IDATA,512,IDFSEC+M,INODE)
              CALL EXIT
              END


!
C ---------------------------------------------------------------
C "BLANKZ.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: BLZ
C
C ---------------------------------------------------------------
```

```
C
      PROGRAM BLANKZ
C
C CALLED BY MACRO "BLZ".  BLANKS SEVERAL SELECTED RANGES OF AN
C ABSORPTION SPECTRUM.  THE BASELINES OF UNBLANKED SEGMENTS ARE
C ADJUSTED TO AVOID SUDDEN OFFSETS IN THE Y-AXIS AT RANGE
C LIMITS.  THE MAIN PURPOSE OF THIS PROGRAM IS TO EXTRACT THE
C BANDS OF A PARTICULAR MOLECULE FROM ALL OTHER BANDS IN A
C SPECTRUM (E.G. THE SPECTRUM OF AN ISOTOPE OF HYDRAZINE CAN BE
C EXTRACTED FROM THE SPECTRUM OF AN ISOTOPIC MIXTURE AND THEN
C PLOTTED FOR A JOURNAL PUBLICATION).
C
C THE INPUT CM-1 RANGES MUST BE INSERTED INTO DATA FILE
C "BLANK.DAT" AS FOLLOWS:
C
C 1) ENTER THE # OF CM-1 RANGES TO BE BLANKED (I4 FORMAT).
C 2) ENTER THE CM-1 RANGES IN ASCENDING ORDER OF CM-1 (2F7).
C 3) REPEAT STEPS 1 & 2 FOR ADDITIONAL SPECTRA.
C
      DIMENSION IDATA(512)
      REAL LXF,NXTFRQ
      OPEN (12,FILE='BLANK.DAT',FORM='FORMATTED',STATUS='OLD')
      DATA R /0.016204542/, ZERO /262144/
C
C READ FTIR PARAMETERS:
C
      IDFN=   IRVAL(14022,0)
      NSECS=  IRVAL(14001,0)
      INODE=  IRVAL(13004,0)
      NTP256= IRVAL(14002,0)
      ID  =   IRVAL(13764,0)
C
      IDFSEC=IDFN*NSECS+88-1
      PPWVN=R*NTP256
      IF (ID.EQ.1) GO TO 18
C
C READ PAST ALL INPUT DATA PRECEDING THE DESIRED DATA:
C
      DO 15 I=1,ID-1
      READ(12,1001) NRANGE
      DO 12 J=1,NRANGE
12    READ(12,2001) TRASH1,TRASH2
15    CONTINUE
C
18    READ(12,1001) NRANGE
      READ(12,2001) FRQ0,FXF
C
C ***************************************************************
C BEGIN CM-1 RANGE LOOP:
C
      DO 500 K=1,NRANGE
      IF (K.NE.NRANGE) READ(12,2001) LXF,NXTFRQ
      ICOUNT=0
```

```
C
C COMPUTE WORD INDICES FOR THE BEGINNING OF THE BLANKED RANGE
C (NBEGIN), THE BEGINNING OF THE UNBLANKED RANGE (NPKI), AND
C THE END OF THE UNBLANKED RANGE (NPKF):
C
      NPKI=1+PPWVN*FXF
      NPKF=1+PPWVN*LXF
      NBEGIN=1+PPWVN*FRQ0
C
C COMPUTE SECTOR AND ARRAY INDICES CORRESPONDING TO ABOVE WORDS
C
        IISEC=NBEGIN/512+1
        IPISEC=NPKI/512+1
        IFSEC=NPKF/512+1
      LPKLOC=NPKF-512*(IFSEC-1)
      IPKLOC=NPKI-512*(IPISEC-1)
      LOCBEG=NBEGIN-512*(IISEC-1)
C
        IF (K.EQ.NRANGE) IFSEC=IPISEC
        IF (K.EQ.NRANGE) GO TO 27
C
C COMPUTE THE SLOPE AND INTERCEPT OF THE BASELINE CORRECTION:
C
      CALL IRTISK(IDATA,512,IDFSEC+IFSEC,INODE)
      LBASE=IDATA(LPKLOC)-ZERO
      IF (IFSEC.NE.IPISEC) CALL IRTISK(IDATA,512,IDFSEC+IPISEC,
     1                                 INODE)
      IBASE=IDATA(IPKLOC)-ZERO
      ZB=IDATA(IPKLOC)
      SLOPE=(LBASE-IBASE)/(1.0*(NPKF-NPKI))
C
C ***************************************************************
C PROCESS SECTORS CORRESPONDING TO THE CURRENT CM-1 RANGE:
C
27    DO 100 I=IISEC,IFSEC
      IF (I.NE.IISEC.OR.IISEC.NE.IPISEC.OR.K.EQ.NRANGE)
     1    CALL IRTISK (IDATA,512,IDFSEC+I,INODE)
      JI=1
      JL=512
      IF (I.EQ.IISEC)  JI=LOCBEG
      IF (I.EQ.IPISEC) JL=IPKLOC
C
C CASE 1: (I < IPISEC); SECTOR PRECEDES UNBLANKED RANGE; DO
C                       BLANKING ONLY.
C CASE 2: (I = IPISEC); SECTOR CONTAINS THE START OF THE
C                       UNBLANKED RANGE; DO BLANKING AND THEN
C                       BASELINE CORRECTIONS.
C CASE 3: (I > IPISEC); SECTOR BEGINS BEYOND THE START OF THE
C                       UNBLANKED RANGE; DO ONLY BASELINE
C                       CORRECTIONS.
C
      IF (I.GT.IPISEC) GO TO 55
29    DO 30 J=JI,JL
```

```
30    IDATA(J)=ZERO
      IF (I.NE.IPISEC.OR.K.EQ.NRANGE) GO TO 70
      JI=IPKLOC+1
55    IF (I.GT.IPISEC) JI=1
      JL=LPKLOC
      IF (I.NE.IFSEC) JL=512
      IF (JI.GT.JL) GO TO 70
      DO 60 J=JI,JL
      ICOUNT=ICOUNT+1
60    IDATA(J)=IDATA(J)*ZERO/(ZB+SLOPE*ICOUNT)
70    CALL IWTISK(IDATA,512,IDFSEC+I,INODE)
100   CONTINUE
C *****************************************************************
C
      FRQ0=LXF
      FXF=NXTFRQ
500   CONTINUE
1001  FORMAT(I4)
2001  FORMAT(2F7.2)
      CALL EXIT
      END
```

```
!
C ---------------------------------------------------------------
C "EMPFIL.FOR"
C
C CALLS:   FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: EMP
C
C ---------------------------------------------------------------
C
      PROGRAM EMPFIL
C
C "EMPFIL.FOR" IS CALLED BY MACRO "EMP".  IT CHECKS THE FSB OF
C  FTIR FILE "DFN" TO SEE WHETHER THE FILE IS VACANT OR NOT, &
C SETS FTIR PARAMETER "CMP" TO 0 (FILLED) OR 99 (VACANT).
C
      INTEGER IW(512)
C
      IDFN  = IRVAL( 14022, 0 )
      NSECS = IRVAL( 14001, 0 )
      INODE = IRVAL( 13004, 0 )
C
      CALL IRTISK( IW, 512, NSECS * IDFN + 88 + 87, INODE )
      ICMP = 0
      IF ( IW(2). NE. 342225 )  THEN
           ICMP = 99
           PRINT *,'FILE #', IDFN, 'WAS VACANT'
```

```
      ENDIF
      CALL IRPUT( 13761, 0, ICMP )
      CALL EXIT
      END



!
C -------------------------------------------------------------
C "FSBTIT.FOR"
C
C SUBROUTINE OF "PLOTFT.FOR"
C
C -------------------------------------------------------------
      SUBROUTINE FSBTIT( IFILE,TITYPE,NSECS,INODE,IDATA,TITLE,
     1                   LETITL )
C
C READS THE TITLE (TITYPE=0) OR MACRO DESCRIPTOR (TITYPE=1) FROM
C THE FILE STATUS BLOCK OF FTIR SCRATCH FILE # "IFILE".  THE
C FSB IS LOCATED USING THE INPUT VALUES FOR # OF SECTORS PER
C FILE (NSECS) AS WELL AS THE FTIR "INODE" VALUE.  "IDATA" IS
C AN ARRAY USED FOR TEMPORARY DATA STORAGE.
C
C THE OUTPUT IS THE TITLE AND THE # OF LETTERS IN THE TITLE.
C
      INTEGER TITLE(88),IDATA(512),TITYPE
C
            ISEC=(IFILE+1)*NSECS+88-1
            CALL IRTISK(IDATA,512,ISEC,INODE)
            NBLANK=0
            LETITL=0
C
            IF (TITYPE.EQ.0) THEN
                  JMIN=68
                  JMAX=107
               ELSE
                  JMIN=145
                  JMAX=232
            ENDIF
C
C CHARACTER CODES FOR FSB CHARACTERS:
C
C 0 OR 1 :  NULL
C 141    :  'RETURN' CHARACTER IN FTIR FILE TITLES
C 160    :  BLANK
C 166    :  &
C 176-185:  NUMERALS 0-9
C 193-218:  A TO Z
C
C THE TITLE IS TERMINATED WHEN 0, 1, 141, 166, OR 3 SUCCESSIVE
C 160'S ARE ENCOUNTERED (SEE ABOVE CODE TABLE).
```

```
C
      DO 101 J=JMIN,JMAX
             IF (IDATA(J).LE.0.OR.IDATA(J).EQ.166.OR.
     1           IDATA(J).EQ.141)   GO TO 201
             TITLE(J+1-JMIN)=IDATA(J)
             LETITL=LETITL+1
             IF (IDATA(J).EQ.160) NBLANK=NBLANK+1
             IF (IDATA(J).NE.160) NBLANK=0
             IF (NBLANK.GT.2)                              GO TO 201
101          CONTINUE
201          LETITL=LETITL-NBLANK
             RETURN
             END




!
C ---------------------------------------------------------------
C "FSPRN.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: FSP
C
C ---------------------------------------------------------------
C
C PRINTS A SECTOR OF FTIR SCRATCH FILE DATA.
C
      PROGRAM FSPRN
      INTEGER IW(512)
             IDFN  =IRVAL(14022,0)
             NSECS =IRVAL(14001,0)
             INODE =IRVAL(13004,0)
             ISEC  =IRVAL(14177,0)
             CALL IRTISK(IW,512,NSECS*IDFN+ISEC+87,INODE)
             IEND=-4
      DO 201 J=1,4
             WRITE(2,1000) IDFN,ISEC
             WRITE(2,3000)
             ISTART=IEND+5
             IEND=IEND+150
             IF (J.EQ.4) IEND=506
      DO 101 I=ISTART,IEND,5
101          WRITE(2,2000) I,IW(I),IW(I+1),IW(I+2),
     1                      IW(I+3),IW(I+4)
             IF (J.EQ.4) THEN
                 WRITE(2,2000) 511,IW(511),IW(512)
             ELSE
                 PRINT *,'TYPE <CR> TO CONTINUE:'
                 READ *,I
             ENDIF
```

```
201          CONTINUE
1000  FORMAT(' ','FILE = ',I3,'        SECTOR = ',I3)
2000  FORMAT(' ',I8,10X,5I8)
3000  FORMAT('0',' ')
      CALL EXIT
      END
```

```
!
C ------------------------------------------------------------
C "FSWR.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: FSW
C
C ------------------------------------------------------------
C
C THIS PROGRAM CHANGES A SINGLE WORD IN THE STATUS BLOCK OF AN
C FTIR SCRATCH FILE.
C
      PROGRAM FSWR
      INTEGER IW(512),WORD
              INODE = IRVAL(13004,0)
              IWORD = IRVAL(13762,0)
              WORD  = IRVAL(13763,0)
              NSECS = IRVAL(14001,0)
              IDFN  = IRVAL(14022,0)
              CALL IRTISK( IW, 512, NSECS*(IDFN+1)+87, INODE )
              IW(IWORD) = WORD
              CALL IWTISK( IW, 512, NSECS*(IDFN+1)+87, INODE )
      CALL EXIT
      END
```

```
!
C ------------------------------------------------------------
C "FTPARM.FOR"
C
C SUBROUTINE OF MANY FTIR PROGRAMS
C ------------------------------------------------------------
C
      SUBROUTINE FTPARM(IHENE,RFXF,RLXF,FRQMIN,FRQMAX,IISEC,
     1                  IFSEC,INDXSP,INDXEP,PPWVN)
C ************************************************************
C
C PURPOSE OF SUBROUTINE:
```

```
C      COMPUTE SPECTRAL RANGE PARAMETERS.
C
C INPUT:
C
C IHENE         : HENE LASER CM-1 MULTIPLIED BY 32  (I.E. THE
C                 WORD STORED IN DECIMAL LOCATION 332 OF FSB).
C RFXF,RLXF     : INITIAL AND FINAL WAVENUMBERS OF THE SPECTRAL
C                 REGION UNDER CONSIDERATION.
C
C OUTPUT:
C
C FRQMIN,FRQMAX: RFXF AND RLXF ARRANGED IN ASCENDING ORDER.
C IISEC,IFSEC   : RELATIVE INITIAL & FINAL SECTORS CORRESPONDING
C                 TO FRQMIN & FRQMAX (WITH SECTOR 1 DEFINED AS
C                 BEGINNING AT 0 CM-1 OF THE CURRENT SPECTRUM).
C INDXSP,INDXEP: RELATIVE INITIAL AND FINAL WORDS CORRESPONDING
C                 TO FRQMIN AND FRQMAX (EACH REFERENCED TO THE
C                 START OF THE SECTOR IN WHICH IT IS LOCATED).
C PPWVN         : RATIO OF WORD RANGE TO WAVENUMBER RANGE.
C ***********************************************************C
C
      NTP256= IRVAL(14002,0)
      LASWVN= IHENE/32
      R=0.016204542
      IF (LASWVN.EQ.15798) R=0.016204008
      PPWVN= R * NTP256
      FRQMIN=RFXF
      FRQMAX=RLXF
      IF (RLXF.LT.RFXF) FRQMIN=RLXF
      IF (RLXF.LT.RFXF) FRQMAX=RFXF
C
C IFWORD IS OBTAINED BY TRUNCATION.  IIWORD IS OBTAINED BY
C TRUNCATION FOLLOWED BY ADDING AN EXTRA 1.
C
      IIWORD=2+INT(PPWVN*FRQMIN)
      IISEC =(IIWORD-1)/512+1
      INDXSP=IIWORD+(1-IISEC)*512
      IFWORD=1+INT(PPWVN*FRQMAX)
      IFSEC =(IFWORD-1)/512+1
      INDXEP=IFWORD+(1-IFSEC)*512
      RETURN
      END



!
C ------------------------------ ------------------------------
C "INTGRL.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: ITG
```

```
C
C ---------------------------------------------------------------
C
      PROGRAM INTGRL
C
C "INTGRL.FOR" IS USED IN CONJUNCTION WITH MACRO "ITG" TO
C INTEGRATE SELECTED CM-1 RANGES OF AN ABSORBANCE FILE.  THE
C INPUT CM-1 RANGES MUST BE INSERTED INTO DATA FILE
C "INTSEG.DAT" AS FOLLOWS:
C
C 1) ENTER THE # OF CM-1 RANGES TO BE INTEGRATED (I4 FORMAT).
C
C 2) ENTER A BAND ID # (E.G. NORMAL MODE #) & A PAIR OF CM-1
C    RANGES ON EACH NEW LINE (I5,2F7 FORMAT).
C
C 3) REPEAT STEPS 1 & 2 FOR ADDITIONAL SPECTRA.
C
C ***************************************************************
C "INTGRL.FOR" IS CALLED BY MACRO "ITG" & IS WITHIN A MACRO
C DO LOOP.  EXCEPT FOR THE FIRST, SECOND, AND LAST ITERATIONS
C OF THIS PROGRAM, EACH ITERATION CONSISTS OF:
C
C     1) READING FROM THE DATA FILE (UNIT 12) THE CM-1 RANGE
C        THAT HAS JUST BEEN INTEGRATED IN THE MACRO ROUTINE,
C        AND THEN PRINTING THE INTEGRATED INTENSITY FOR THIS
C        RANGE.
C
C     2) PUTTING THE NEXT CM-1 RANGE INTO THE PARAMETER
C        STORAGE AREA WHERE IT CAN BE ACCESSED BY THE MACRO.
C
C FOR ITERATIONS 1 AND 2, THE FIRST STEP IS SKIPPED. ITERATION
C 1 DEALS WITH THE REFERENCE PEAK, AND 2 DEALS WITH THE 1ST
C CM-1 RANGE.  FOR THE LAST ITERATION, STEP 2 IS SKIPPED.
C
C ***************************************************************
C ***************************************************************
      INTEGER QIT
      REAL ITG,LXF
      DIMENSION RFXF(50),RLXF(50),NVMODE(50)
      OPEN (12,FILE='INTSEG.DAT',FORM='FORMATTED',STATUS='OLD')
C
C ***************************************************************
C RETRIEVE THE MACRO PARAMETERS SPECIFYING THE SET OF CM-1
C RANGES TO BE USED (ID), AND THE UPPER MACRO DO LOOP LIMIT
C (QIT).  QIT IS 1 UNIT LARGER THAN THE INDEX OF THE FINAL CM-1
C RANGE TO BE PRINTED.
C
      ID  = IRVAL(13764,0)
      QIT = IRVAL(14222,0)
C
C OBTAIN THE CURRENT(I=VI1) AND INITIAL(IFIRST=VI3) MACRO CM-1
C LOOP INDICES. "I" CORRESPONDS TO THE CM-1 RANGE THAT WILL
C SUBSEQUENTLY BE INTEGRATED BY THE MACRO. IFIRST IS THE INDEX
```

```
C OF THE FIRST CM-1 RANGE TO BE PRINTED.
C
      I      = IRVAL(13763,0)
      IFIRST = IRVAL(13765,0)
      IROUTE = 0
C
C ****************************************************************
C READ DATA FILE.  THE FIRST ID-1 SETS OF DATA ARE READ BUT
C ARE OVERWRITTEN BY SET ID.
C
      DO 60 K = 1, ID
            READ (12,5000) NLIST
      DO 50 J = 1, NLIST
50          READ(12,4000) NVMODE(J), RFXF(J), RLXF(J)
60          CONTINUE
C
            IF ( I. GT. IFIRST )                          GO TO 180
            IF ( I. EQ. IFIRST )                          GO TO 90
C ****************************************************************
C PRINT HEADING.
C
            WRITE (2,1000)
C
            I      = IRVAL(14023,0)
90          IROUTE = 1
                                                          GO TO 180
C
C ****************************************************************
C READ THE INTEGRATED ABSORPTION VALUE WHICH WAS STORED DURING
C THE PREVIOUS ITERATION OF THE MACRO (SKIP THIS STEP ON THE
C FIRST ITERATION OF THIS FORTRAN PROGRAM):
C
100         ITG = RVAL(14062,0)
C
C ****************************************************************
C SET UP PRINTER OUTPUT:
C
130         REF = RVAL(13766,0)
            REL = ITG / REF
C
            WRITE(2,2000) FXF, LXF, ITG, REL, NMODE
            IF ( I. EQ. QIT) WRITE (2,3000)
            IF ( I. EQ. QIT)                              GO TO 200
C
C ****************************************************************
C SET CM-1 LIMITS FOR PRINTING (IROUTE=0) OR FOR NEXT
C INTEGRATION (IROUTE=1).
C
          IROUTE = 1
180       J      = I - 1 + IROUTE
          FXF    = RFXF(J)
          LXF    = RLXF(J)
          NMODE  = NVMODE(J)
```

```
          IF (IROUTE) 100,100,190
C
C ***************************************************************
C STORE NEW INTEGRATION LIMITS IN THE PARAMETER STORAGE AREA
C FOR SUBSEQUENT RETRIEVAL BY MACRO ITG.
C
190       FI = FXF
          FF = LXF
          CALL RPUT( 14135, 0, FI )
          CALL RPUT( 14213, 0, FF )
200       CALL EXIT
1000  FORMAT(' ',20X,'FXF',6X,'LXF',8X,'I',7X,'IREL',3X,'MODE #
     1')
2000  FORMAT(20X,2(F6.1,3X),2(F6.3,3X),I4)
3000  FORMAT('0',' ')
4000  FORMAT(I5,2F7.1)
5000  FORMAT(I4)
      END




!
C ---------------------------------------------------------------
C "LETTRS.FOR"
C
C CALLS: 1)  "GPLOT.LIB" SYSTEM PLOTTING SUBROUTINES
C        2)  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: LTR
C
C ---------------------------------------------------------------
C
      PROGRAM LETTRS
C
C THIS PROGRAM SENDS CHARACTERS FROM THE KEYBOARD TO THE
C PLOTTER.  IT IS CALLED BY MACRO 'LTR'.
C
      CHARACTER ANYKEY*10,STRING(80)*1
C
              CALL PLOTS(3)
              NCHTOT=0
              WRITE(2,1100)
              WRITE(2,1500)
              READ(2,*) CHRSIZ
              WRITE(2,400)
              WRITE(2,1500)
              READ(2,*) ANGLE
      DO 101 J=1,1000
1             WRITE(2,600)
              WRITE(2,700)
              WRITE(2,800)
```

```
             WRITE(2,900)
             WRITE(2,1000)
             WRITE(2,500)
             WRITE(2,1500)
            READ(2,200) STRING
            NLETRS=0
      DO 11 I=1,80
            IC=ICHAR(STRING(I))
            IF (IC.EQ.33)                                    GO TO 21
11          NLETRS=NLETRS+1
            WRITE(2,1300)
                                                             GO TO  1
21          WRITE(2,1400) NLETRS
            IF (NLETRS.EQ.0)                                 GO TO 999
            IF (ICONT.EQ.0) THEN
               WRITE(2,1200)
               READ (2,100) ANYKEY
               ENDIF
            IF (ICHAR(STRING(NLETRS+2)).EQ.33) THEN
                 ICONT=1
                 NCHTOT=NCHTOT+NLETRS
             ELSE
                 ICONT=0
             ENDIF
            C=COS(ANGLE*0.017453292)
            S=SIN(ANGLE*0.017453292)
            XSHIFT=  CHRSIZ*( (1-ICONT)* 1.3*S + ICONT*NLETRS*C)
            YSHIFT=  CHRSIZ*( (1-ICONT)*-1.3*C + ICONT*NLETRS*S)
            CALL SYMBOL(0.0,0.0,CHRSIZ,STRING,ANGLE,NLETRS)
C
C IF THE CURRENT LINE IS FINISHED (I.E. ICONT=0) MOVE TO THE
C NEXT LINE IN THE DIRECTION PERPENDICULAR TO THE CURRENT LINE.
C (NOTE: "CALL PLOT" DOES NOTHING IF ICONT=1.)
C
            CALL PLOT(XSHIFT,YSHIFT,-3)
C
C IF ICONT=0, MOVE BACK TO THE POSITION OF THE 1ST CHARACTER OF
C THE NEXT LINE IN THE DIRECTION PARALLEL TO THE CURRENT
C LINE.
C
            IF (ICONT.EQ.0.AND.NCHTOT.NE.0) THEN
                XSHIFT= -CHRSIZ*NCHTOT*C
                YSHIFT= -CHRSIZ*NCHTOT*S
                NCHTOT=0
                CALL PLOT(XSHIFT,YSHIFT,-3)
                ENDIF
101         WRITE(2,500)
999         CALL PLOT(0,0,999)
100   FORMAT(A10)
200   FORMAT(80A1)
300   FORMAT(F10.0)
400   FORMAT('0','ENTER ANGLE OF LETTERS (0,90,180, OR 270): ')
500   FORMAT('0','         *         *         *         *
```

```
     /   *         *         *         *')
600   FORMAT('0','TYPE THE CHARACTERS TO BE PLOTTED (MAX OF 80
     / PER LINE);')
700   FORMAT(' ',' END THE STRING WITH EITHER:')
800   FORMAT(' ','    A) AN EXCLAMATION MARK TO EXECUTE [CR] ON
     / THE PLOTTER.')
900   FORMAT(' ','    B) 2 EXCLAMATION MARKS TO CONTINUE THE
     / LINE LATER.')
1000  FORMAT('0','PUT AN EXCLAMATION MARK IN COLUMN #1 TO
     / DISCONTINUE THE PROGRAM:')
1100  FORMAT(' ','ENTER THE CHARACTER SIZE IN INCHES')
1200  FORMAT('0','POSITION THE PLOTTER PEN; THEN TYPE [CR]')
1300  FORMAT('0','ERROR: NO EXCLAMATION MARK FOUND')
1400  FORMAT(' ','# OF LETTERS IN STRING =',I3)
1500  FORMAT(' ','')
      CALL EXIT
      END



!
C -------------------------------------------------------------
C "MATINV.FOR"
C
C SUBROUTINE OF "SPLINE.FOR"
C -------------------------------------------------------------
C
      SUBROUTINE MATINV(N,A)
      DIMENSION A(10,10),IP(10,3)
      D=1.0
      DO 51 J=1,N
51          IP(J,3)=0
      DO 901 I=1,N
            AM=0.0
      DO 201 J=1,N
            IF (IP(J,3).EQ.1) GO TO 201
      DO 101 K=1,N
            IF (IP(K,3).EQ.1) GO TO 101
            IF (AM.GE.ABS(A(J,K))) GO TO 101
            IR=J
            IC=K
            AM=ABS(A(J,K))
101         CONTINUE
201         CONTINUE
            IF (AM.LE.1.0E-30) GO TO 1201
            IP(IC,3)=1
            IP(I,1)=IR
            IP(I,2)=IC
            IF (IR.EQ.IC) GO TO 351
      DO 301 L=1,N
            SW=A(IR,L)
```

```
                A(IR,L)=A(IC,L)
301             A(IC,L)=SW
351             PV=A(IC,IC)
                D=D*PV
                A(IC,IC)=1.0
      DO 401 L=1,N
401             A(IC,L)=A(IC,L)/PV
      DO 601 L1=1,N
                IF (L1.EQ.IC) GO TO 601
                T=A(L1,IC)
                A(L1,IC)=0.0
      DO 501 L=1,N
501             A(L1,L)=A(L1,L)-A(IC,L)*T
601             CONTINUE
901             CONTINUE
                NS=0
      DO 1101 I=1,N
                L=N-I+1
                IF (IP(L,1).EQ.IP(L,2)) GO TO 1101
                JR=IP(L,1)
                JC=IP(L,2)
                NS=NS+1
      DO 1001 K=1,N
                 SW=A(K,JR)
                 A(K,JR)=A(K,JC)
1001             A(K,JC)=SW
1101             CONTINUE
1201             RETURN
                 END
```

```
!
C ---------------------------------------------------------------
C "PLOTFT.FOR"
C
C CALLS: 1)  "GPLOT.LIB" SYSTEM PLOTTING SUBROUTINES
C        2)  FTIR SYSTEM SUBROUTINES
C        3)  "FSBTIT.FOR"
C        4)  "AXIS2.FOR"
C
C CALLING MACROS: PLI & PLC
C
C AUXILIARY PROGRAMS: "PLPARW.FOR" & "PLPARR.FOR"
C ---------------------------------------------------------------
C
      PROGRAM PLOTFT
C
C THIS PROGRAM IS CALLED BY MACROS 'PI0' & 'PLC'.  IT PRODUCES
C A SINGLE PLOT USING DATA INPUT FROM FTIR PARAMETERS.
C
```

```
C ****************************************************************
C THE DIMENSIONS OF THE X AND Y ARRAYS ARE 512*SECBLK+2; A MAX
C OF 10 SECTORS ARE PROCESSED EACH TIME SUBROUTINE 'LINE' IS
C CALLED.
C
C
      INTEGER   TITLE(88),LTABSC(15),LETORD(15),IDATA(512),
     $          PENDAT,PENAX,PENTIT,PLTROT,AUTSCA,
     $          ADECDG,WDECDG,ATKRAT,WTKRAT,SECBLK,
     $          SECRSM,WRDRSM,RESUME
      REAL      X(5122),Y(5122)
      CHARACTER ABSCLT(30)*1,ORDLET(30)*1
      DATA      RESUME/0/,SECBLK/10/,
     $          ABSCLT
     $          /'W','A','V','E','N','U','M','B','E','R','S'
     $          ,'N','A','N','O','M','E','T','E','R','S'/,
     $          ORDLET
     $     /'A','B','S','O','R','B','A','N','C','E'
     $     ,'T','R','A','N','S','M','I','T','T','A','N','C','E'/
C
C ****************************************************************
C READ INPUT FROM FTIR PARAMETER STORAGE:
C
      INODE =IRVAL(13004,0)
      ITER  = RVAL(13702,0)
      ASIZNM=IRVAL(13710,0)*.01
      AUTSCA=IRVAL(13713,0)
      DSTNUM=IRVAL(13714,0)*.01
      WSIZNM=IRVAL(13715,0)*.01
      OFFSET=IRVAL(13731,0)*.01
      SZMJTC=IRVAL(13732,0)*.01
      SIZLET=IRVAL(13733,0)*.01
      SIZTIT=IRVAL(13735,0)*.01
      AANGAX=IRVAL(13736,0)
      AANGNM=IRVAL(13750,0)
      WTKRAT=IRVAL(13751,0)
      ATKRAT=IRVAL(13752,0)
      PLTROT=IRVAL(13753,0)
      PENDAT=IRVAL(13760,0)
      IWAXON=IRVAL(13762,0)
      IAAXON=IRVAL(13763,0)
      ITITON=IRVAL(13764,0)
      PENTIT=IRVAL(13765,0)
      WJSTNM= RVAL(13772,0)
      AJSTNM= RVAL(13774,0)
      VF4   = RVAL(13776,0)
      NSECS =IRVAL(14001,0)
      NTP   =IRVAL(14002,0)*256
      DSTLET=IRVAL(14006,0)*.01
      WDECDG=IRVAL(14012,0)
      WNMBEG= RVAL(14017,0)
      IDFN  =IRVAL(14022,0)
      IOVRLP=IRVAL(14023,0)
```

```
      WANGLT=IRVAL(14027,0)
      NFILAS=IRVAL(14030,0)
      ASTART= RVAL(14031,0)
      AEND  = RVAL(14033,0)
      AANGLT=IRVAL(14035,0)
      WANGNM= RVAL(14062,0)
      TCSZRT= RVAL(14064,0)
      ADECDG=IRVAL(14072,0)
      ANMSPC= RVAL(14120,0)
      WSTART= RVAL(14135,0)
      WTITCO= RVAL(14153,0)
      ANMBEG= RVAL(14161,0)
      WAXSPN= RVAL(14172,0)
      WNMSPC= RVAL(14174,0)
      PENAX =IRVAL(14177,0)
      APN00 = RVAL(14205,0)
      AAXSPN= RVAL(14207,0)
      ATITCO= RVAL(14211,0)
      WEND  = RVAL(14213,0)
      WPN0  = RVAL(14215,0)
      WANGAX=IRVAL(14221,0)
      IQIT  =IRVAL(14222,0)
C
C CALCULATE THE Y SPAN (INCHES) OF THE CURRENT PLOT:
C
      IF (IOVRLP.EQ.1) AISPAN = AAXSPN + (1 - IQIT) * VF4
      IF (IOVRLP.EQ.0) AISPAN = (AAXSPN + (1 - IQIT)*VF4) / IQIT
      IF (VF4.LT.-10)  AISPAN = AAXSPN
C
C CALCULATE THE PEN POSITION OF THE CURRENT PLOT ORIGIN:
C
      IF ( IOVRLP. EQ. 1 ) APN0 = ITER * VF4 + APN00
      IF ( IOVRLP. EQ. 0 ) APN0 = ITER * ( AISPAN + VF4) + APN00
      IF (PLTROT.EQ.0) THEN
          XPN0 = WPN0
          YPN0 = APN0
       ELSE
          XPN0 = APN0
          YPN0 = WPN0
       ENDIF
C
      IF (WEND.GT.WSTART.AND.WNMSPC.LT.0) WNMSPC= -WNMSPC
      IF (WEND.LT.WSTART.AND.WNMSPC.GT.0) WNMSPC= -WNMSPC
      IF (AEND.GT.ASTART.AND.ANMSPC.LT.0) ANMSPC= -ANMSPC
      IF (AEND.LT.ASTART.AND.ANMSPC.GT.0) ANMSPC= -ANMSPC
C ************************************************************
C
C 'OFFSET' IS THE MINIMUM ALLOWED DISTANCE BETWEEN THE BASELINE
C AND THE CM-1 AXIS IN INCHES.  IT IS USED TO KEEP THE BASELINE
C AND THE CM-1 AXIS FROM COINCIDING.  'RNGMLT' IS THE RANGE
C EXPANSION FACTOR COMPUTED FROM 'OFFSET'.  THE EXPANDED RANGE
C IS SUBTRACTED FROM THE MAX ABSORBANCE TO OBTAIN A REVISED
C LOWER ABSORBANCE AXIS LIMIT 'ASTART'.
```

```
C
       IF (AUTSCA.EQ.1) THEN
           RNGMLT = AISPAN/(AISPAN-OFFSET)
           ASTART = AEND - RNGMLT*(AEND-ASTART)
           ANMBEG = ASTART
           ANMSPC = (AEND-ASTART)/AISPAN
           ENDIF
C
C INITIALIZE THE PLOTTER & READ THE FILE STATUS BLOCK:
C
      CALL PLOTS(3)
      CALL FSBTIT(IDFN,IT,NSECS,INODE,IDATA,TITLE,LETITL)
C
      NX=-524288
      IF (PENAX.NE.1) CALL NEWPEN(PENAX)
      IPEN=PENAX
C
C ****************************************************************
C DRAW ABSORBANCE AXIS:
C
      IF (IAAXON.EQ.0)                                    GO TO 101
            IT = ITITON - 1
            IF (IDATA(9).EQ.0)  THEN
                ILOW   = 11
                NLORD  = 13
             ELSEIF (IDATA(10).EQ.0) THEN
                ILOW   = 1
                NLORD  = 10
             ELSE
                NLORD  = 0
             ENDIF
            J = 0
            IF (NLORD.EQ.0)                               GO TO 93
      DO 91  I = ILOW, ILOW + NLORD - 1
            J = J + 1
91          LETORD(J) = ICHAR(ORDLET(I))
C
93    IF (ADECDG.GE.10) ADECDG =  2 - ALOG10(AEND)
C
C FOR COMPARISON PLOTS, THE Y-AXIS IS DRAWN ONLY ONCE.
C THUS, IN THIS CASE, THE Y AXIS IS DRAWN TO THE FULL LENGTH
C "AAXSPN" RATHER THAN THE INDIVIDUAL PLOT LENGTH "AISPAN".
C
      AXSPAN = AISPAN
      IF (AUTSCA.EQ.1.AND.IOVRLP.EQ.1) AXSPAN = AAXSPN
C
      CALL AXIS2 (ASTART,   AEND,   XPN0,   YPN0, AXSPAN,
     1            AANGAX, SZMJTC, ATKRAT, TCSZRT, ANMBEG,
     2            ANMSPC, ADECDG, ASIZNM, DSTNUM, AJSTNM,
     3            AANGNM, LETORD, NLORD, SIZLET, DSTLET,
     4            0.0   ,AANGLT)
C
C ****************************************************************
```

```
C DRAW WAVENUMBER AXIS:
C
101   IF (IWAXON.EQ.0)                                        GO TO 201
            IF (IDATA(11).EQ.0) THEN
                  ILOW   = 12
                  NLABSC = 10
               ELSE
                  ILOW   = 1
                  NLABSC = 11
               ENDIF
            J = 0
      DO 111 I = ILOW, ILOW + NLABSC - 1
            J = J + 1
111         LTABSC(J) = ICHAR(ABSCLT(I))
      CALL AXIS2 (WSTART,   WEND,   XPN0,   YPN0, WAXSPN,
     1            WANGAX, SZMJTC, WTKRAT, TCSZRT, WNMBEG,
     2            WNMSPC, WDECDG, WSIZNM, DSTNUM, WJSTNM,
     3            WANGNM, LTABSC, NLABSC, SIZLET, DSTLET,
     4            0.0   ,WANGLT)
C
C ****************************************************************
C PRINT FILE TITLE ON PLOT IF SUCH PRINTING WAS REQUESTED.
C
201         IF (ITITON.EQ.0)                                    GO TO 235
            IF (PENTIT.NE.IPEN) CALL NEWPEN(PENTIT)
            IPEN = PENTIT
C
C     DETERMINE THE PEN LOCATION FOR THE 1ST CHARACTER OF THE
C TITLE.  REDUCE THE CURRENT CHARACTER SIZE IF THE TITLE WILL
C OTHERWISE EXCEED THE X-AXIS SPAN:
C
            IF (VF4.LT.SIZTIT.AND.IOVRLP.EQ.1)
     1          ATITCO=ATITCO + (0.1+SIZTIT)*ITER
            ATITLC = APN0 + AISPAN + ATITCO
            SIZ    = SIZTIT
            WRANGE = ABS(WAXSPN)
            IF (LETITL*SIZTIT.GT.WRANGE) SIZTIT = WRANGE/LETITL
C
C CENTERED TITLE:
C
            WTITLC = WPN0 + 0.5*WAXSPN - 0.5*(LETITL-1)*SIZTIT
C
C NON-CENTERED TITLE:
C
            IF (WTITCO.GE.-0.0001) WTITLC = WPN0 + WTITCO
C
C MATCH THE X,Y PEN AXES WITH THE X,Y PLOT AXES:
C
            XPNTIT = WTITLC*(1-PLTROT) + ATITLC*PLTROT
            YPNTIT = WTITLC*PLTROT + ATITLC*(1-PLTROT)
C
         CALL SYMBOL(XPNTIT,YPNTIT,-SIZTIT,TITLE,WANGAX,LETITL)
C
```

```
C ***************************************************************
C SET PARAMETERS REQUIRED FOR PLOTTING SUBROUTINE 'LINE':
C
235          IF (PENDAT.NE.IPEN) CALL NEWPEN(PENDAT)
C
C COMPUTE VALUES NEEDED FOR LAST 2 ELEMENTS OF X AND Y PLOTTING
C ARRAYS OF SUBROUTINE 'LINE'.
C
             XSTART = WSTART*(1-PLTROT) + ASTART*PLTROT
             YSTART = WSTART*PLTROT     + ASTART*(1-PLTROT)
             WPINCH = (WEND-WSTART)/WAXSPN
             APINCH = (AEND-ASTART)/AISPAN
             XPINCH = WPINCH*(1-PLTROT) + APINCH*PLTROT
             YPINCH = APINCH*(1-PLTROT) + WPINCH*PLTROT
C
C COMPUTE SECTOR LIMITS, WORD LIMITS, AND INTENSITY SCALING
C FACTOR NEEDED FOR READING DATA FROM FTIR SCRATCH FILE:
C
             SCLFCT = 1/2.0**(19.0-IDATA(6))
             IF (IDATA(7).EQ.0) SCLFCT = SCLFCT/IDATA(3)
             IF (IDATA(9).EQ.0) SCLFCT = 100*SCLFCT
             AWEND  = AEND/SCLFCT
             IF (IDATA(11).EQ.0) THEN
                IWL    = IDATA(24)
                ABSCSP = (NTP/2.0-1)/(IDATA(25)-IWL)
                IWORD  = (WSTART-IWL)*ABSCSP + 1
                LWORD  = (WEND  -IWL)*ABSCSP + 1
             ELSE
                BNDWID = 15798/IDATA(17)
                ABSCSP = (NTP/2-1)/BNDWID
                IWORD  = WSTART*ABSCSP + 1
                LWORD  = WEND  *ABSCSP + 1
                IWL    = 0
             ENDIF
             IDIR   = 1
             IF (IWORD.GT.LWORD) IDIR = -1
             IDFSEC = IDFN*NSECS + 88 - 1
             ISEC   = IWORD/512 + 1
             INIWRD = IWORD - 512*(ISEC-1)
             LSEC   = LWORD/512 + 1
             LSTWRD = LWORD - 512*(LSEC-1)
             NLCALL = 1 + IDIR*(LSEC-ISEC)/SECBLK
             ISI    = ISEC
C
C SPECTRAL INTENSITIES ARE READ FROM THE DESIGNATED FTIR SCRATCH
C FILE & TRANSFERRED ALONG WITH THEIR ASSOCIATED CM-1'S INTO
C THE X AND Y PLOTTING ARRAYS.  IF THE SPECTRAL DATA FILE
C EXCEEDS 'SECBLK' SECTORS, THE DATA ARE PROCESSED IN BLOCKS
C CONTAINING SECBLK SECTORS EACH.
C
             CALL PLOT(XPN0,YPN0,-3)
       DO 291 J = 1,NLCALL
             ISL = ISI + (SECBLK-1)*IDIR
```

```
            IF (J.EQ.NLCALL) ISL = LSEC
261         IP = 0
C
C SPECTRAL INTENSITIES ARE READ FROM THE DESIGNATED FTIR SCRATCH
C FILE & TRANSFERRED ALONG WITH THEIR ASSOCIATED CM-1'S INTO
C THE X AND Y PLOTTING ARRAYS:
C
      DO 281 IS = ISI,ISL,IDIR
            NBLANK = 0
            IF (RESUME.EQ.1)                                GO TO 266
            CALL IRTISK(IDATA,512,IDFSEC+IS,INODE)
            IF (IDIR.EQ.1) THEN
                ISTART = 1
                IEND   = 512
            ELSE
                ISTART = 512
                IEND   = 1
            ENDIF
            IF (IS.EQ.ISI.AND.J.EQ.1)    ISTART = INIWRD
            IF (IS.EQ.ISL.AND.J.EQ.NLCALL) IEND = LSTWRD
266         RESUME = 0
      DO 271 I = ISTART,IEND,IDIR
            IP = IP+1
C
C IF BLANKED DATA ARE ENCOUNTERED, SEARCH FOR THE END OF THE
C BLANKED DATA, AND SKIP FURTHER FILLING OF THE SPECTRAL ARRAYS.
C USE "NBLANK" TO COUNT THE # OF BLANKED PTS IN THE CURRENT
C BLANKED REGION; "IBLANK" TO RECORD THE INDEX OF THE 1ST
C BLANKED PT IN THE CURRENT X,Y ARRAYS; AND "IP" TO SPECIFY THE
C # OF PTS IN THE CURRENT BLOCK OF DATA.
C
C Y-AXIS VALUES THAT EXCEED THE SPECIFIED Y-AXIS MAXIMUM ARE
C TREATED AS IF THEY WERE BLANKED PTS.
C
            IF (IDATA(I).EQ.NX.OR.IDATA(I).GT.AWEND) THEN
                IF (NBLANK.EQ.0) IBLANK = IP
                NBLANK = NBLANK+1
C
C IF GOOD DATA ARE FOUND AFTER A BLANKED REGION HAS BEEN
C ENCOUNTERED, SAVE THE SECTOR AND WORD INDICES OF THE START OF
C THE GOOD DATA, AND THEN PLOT THE REGION (IF ANY) THAT
C PRECEDED THE BLANKED REGION.
C
            ELSEIF (NBLANK.NE.0) THEN
                SECRSM = IS
                WRDRSM = I
                IP = IBLANK-1
                IF (IP.GT.0)                                GO TO 285
                IF (IP.LE.0)                                GO TO 287
            ELSE
                ABSCVL = (512*(IS-1)+I-1)/ABSCSP + IWL
                X(IP)  = SCLFCT*IDATA(I)*PLTROT
     $                       + ABSCVL*(1-PLTROT)
```

```
                    Y(IP)   = SCLFCT*IDATA(I)*(1-PLTROT)
     $                        + ABSCVL*PLTROT
                    ENDIF
271           CONTINUE
C
C IF A BLANKED REGION EXTENDS TO THE END OF A BLOCK OF PLOTTING
C DATA, RESET THE BLOCK INDEX TO THE LAST GOOD DATA POINT AND
C THEN PLOT THE DATA.
C
              IF (NBLANK.NE.0) THEN
                  IP = IBLANK-1
                  NBLANK = 0
                  ENDIF
281           CONTINUE
C
C SET THE PEN ORIGIN EQUAL TO THE AXIS ORIGIN & THEN PLOT A
C BLOCK OF DATA.  SINCE THE LAST 2 ELEMENTS OF THE X & Y ARRAYS
C ARE ALWAYS DETERMINED FROM THE OVERALL CM-1 BOUNDARIES RATHER
C THAN THE BLOCK BOUNDARIES, THE PEN ORIGIN IS NOT SHIFTED FOR
C EACH NEW BLOCK.
C
285           X(IP+1) = XSTART
              Y(IP+1) = YSTART
              X(IP+2) = XPINCH
              Y(IP+2) = YPINCH
              IF (IP.GT.1) CALL LINE(X,Y,IP,1,0,2)
C
C IF GOOD DATA FOLLOW BLANKED DATA, RESET INDICES TO WHERE THE
C GOOD DATA BEGIN, AND RESTART FILLING THE SPECTRAL ARRAYS.
C
287           IF (NBLANK.EQ.0)                                GO TO 291
                  ISI    = SECRSM
                  ISTART = WRDRSM
                  RESUME = 1
                                                            GO TO 261
291           ISI = ISL + IDIR
C
C MOVE THE PEN BACK TO THE ORIGINAL ORIGIN AND RESET THE ORIGIN
C AT THAT POINT.  THEN, CLOSE THE SPECTRAL DATA FILE:
C
              CALL PLOT(-XPN0,-YPN0,999)
                                                            GO TO 1000
700     PRINT *,'FILE READ ERROR IN FILE STATUS BLOCK'
                                                            GO TO 1000
800     PRINT *,'FILE READ ERROR DURING READ SKIP'
                                                            GO TO 1000
900     PRINT *,'FILE READ ERROR IN MAIN DATA READ'
1000          CALL EXIT
              END
```

```
!
C ------------------------------------------------------------
C "PLPARR.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: PLI & PLC
C
C READS INPUT DATA FOR "PLOTFT.FOR"
C ------------------------------------------------------------
C
      PROGRAM PLPARR
C
C THIS PROGRAM IS CALLED BY CONDITIONAL MACRO "M49" WHICH IS A
C SUB-MACRO OF BOTH "PI0" & "PLC".  IT READS FTIR PLOT
C PARAMETERS FROM PRE-EXISTING NICOS FILE "PLT.DAT".
C
      CHARACTER X*1
      OPEN(11,FILE='PLT.DAT',FORM='FORMATTED',STATUS='OLD')
C
      READ(11,100) X
      READ(11,101) RFXF
      READ(11,101) RLXF
      READ(11,100) X
      READ(11,101) RLXI
      READ(11,100) X
      READ(11,101) RCXL
      READ(11,100) X
      READ(11,101) RFXL
      READ(11,101) RLYT
      READ(11,100) X
      READ(11,102) ISMN
      READ(11,100) X
      READ(11,102) IXSP
      READ(11,102) IXEP
      READ(11,100) X
      READ(11,102) IWTY
      READ(11,100) X
      READ(11,102) IMNT
      READ(11,100) X
      READ(11,102) IRTR
      READ(11,100) X
      READ(11,101) RLXL
      READ(11,101) RLYA
      READ(11,100) X
      READ(11,102) IPEK
      READ(11,100) X
      READ(11,102) ISRT
      READ(11,102) IRTN
      READ(11,100) X
      READ(11,101) RFCD
      READ(11,102) IRTO
      READ(11,100) X
```

```
      READ(11,102) IXSL
      READ(11,102) IYSL
      READ(11,100) X
      READ(11,102) IRTP
      READ(11,100) X
      READ(11,102) IVI2
      READ(11,100) X
      READ(11,102) INSS
      READ(11,100) X
      READ(11,102) IQIT
      READ(11,100) X
      READ(11,102) IOFN
      READ(11,100) X
      READ(11,101) RVF4
      CALL  RPUT(14135,0,RFXF)
      CALL  RPUT(14213,0,RLXF)
      CALL  RPUT(14017,0,RLXI)
      CALL  RPUT(14174,0,RCXL)
      CALL  RPUT(14172,0,RFXL)
      CALL  RPUT(14207,0,RLYT)
      CALL IRPUT(13713,0,ISMN)
      CALL IRPUT(14025,0,IXSP)
      CALL IRPUT(14026,0,IXEP)
      CALL IRPUT(13710,0,IWTY)
      CALL IRPUT(13731,0,IMNT)
      CALL IRPUT(13753,0,IRTR)
      CALL  RPUT(14215,0,RLXL)
      CALL  RPUT(14205,0,RLYA)
      CALL IRPUT(13760,0,IPEK)
      CALL IRPUT(14221,0,ISRT)
      CALL IRPUT(13736,0,IRTN)
      CALL  RPUT(14062,0,RFCD)
      CALL IRPUT(13750,0,IRTO)
      CALL IRPUT(14027,0,IXSL)
      CALL IRPUT(14035,0,IYSL)
      CALL IRPUT(13751,0,IRTP)
      CALL IRPUT(13764,0,IVI2)
      CALL IRPUT(14004,0,INSS)
      CALL IRPUT(14222,0,IQIT)
      CALL IRPUT(14023,0,IOFN)
      CALL  RPUT(13776,0,RVF4)
100   FORMAT(64A1)
101   FORMAT(5X,F7.1)
102   FORMAT(5X,I5)
999   CALL EXIT
      END



!
```

```
C ------------------------------------------------------------
C "PLPARW.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACROS: PLI & PLC
C
C CREATES AN INPUT DATA FILE FOR "PLOTFT.FOR"
C ------------------------------------------------------------
C
      PROGRAM PLPARW
C
C THIS PROGRAM IS CALLED BY CONDITIONAL MACRO "M48" WHICH, IN
C TURN, IS CALLED BY MACROS "PLI" & "PLC".  IT SAVES FTIR PLOT
C PARAMETERS IN A NICOS FILE FOR LATER USE.
C
      INTEGER*2 ISIZE
      OPEN(11,FILE='PLT.DAT',FORM='FORMATTED',STATUS='UNKNOWN',
     $SIZE=ISIZE)
C
      RFXF = RVAL(14135,0)
      RLXF = RVAL(14213,0)
      RLXI = RVAL(14017,0)
      RCXL = RVAL(14174,0)
      RFXL = RVAL(14172,0)
      RLYT = RVAL(14207,0)
      ISMN =IRVAL(13713,0)
      IXSP =IRVAL(14025,0)
      IXEP =IRVAL(14026,0)
      IWTY =IRVAL(13710,0)
      IMNT =IRVAL(13731,0)
      IRTR =IRVAL(13753,0)
      RLXL = RVAL(14215,0)
      RLYA = RVAL(14205,0)
      IPEK =IRVAL(13760,0)
      ISRT =IRVAL(14221,0)
      IRTN =IRVAL(13736,0)
      RFCD = RVAL(14062,0)
      IRTO =IRVAL(13750,0)
      IXSL =IRVAL(14027,0)
      IYSL =IRVAL(14035,0)
      IRTP =IRVAL(13751,0)
      IVI2 =IRVAL(13764,0)
      INSS =IRVAL(14004,0)
      IQIT =IRVAL(14222,0)
      IOFN =IRVAL(14023,0)
      RVF4 = RVAL(13776,0)
      WRITE(11,100)
      WRITE(11,101) RFXF
      WRITE(11,102) RLXF
      WRITE(11,103)
      WRITE(11,104) RLXI
      WRITE(11,105)
```

```
      WRITE(11,106) RCXL
      WRITE(11,107)
      WRITE(11,108) RFXL
      WRITE(11,109) RLYT
      WRITE(11,110)
      WRITE(11,111) ISMN
      WRITE(11,112)
      WRITE(11,1130) IXSP
      WRITE(11,1140) IXEP
      WRITE(11,1141)
      WRITE(11,1142) IWTY
      WRITE(11,115)
      WRITE(11,1160) IMNT
      WRITE(11,1170)
      WRITE(11,1180) IRTR
      WRITE(11,119)
      WRITE(11,1200) RLXL
      WRITE(11,1210) RLYA
      WRITE(11,1240)
      WRITE(11,1250) IPEK
      WRITE(11,126)
      WRITE(11,1270) ISRT
      WRITE(11,1280) IRTN
      WRITE(11,129)
      WRITE(11,1310) RFCD
      WRITE(11,1320) IRTO
      WRITE(11,1330)
      WRITE(11,1340) IXSL
      WRITE(11,1350) IYSL
      WRITE(11,1360)
      WRITE(11,1370) IRTP
      WRITE(11,1380)
      WRITE(11,1390) IVI2
      WRITE(11,1400)
      WRITE(11,1410) INSS
      WRITE(11,1420)
      WRITE(11,1430) IQIT
      WRITE(11,1440)
      WRITE(11,1450) IOFN
      WRITE(11,1480)
      WRITE(11,1490) RVF4
100   FORMAT('WAVENUMBERS OF 1ST & LAST DATA PTS:')
101   FORMAT('FXF  ',F7.1)
102   FORMAT('LXF  ',F7.1)
103   FORMAT('1ST TIC LABEL ON CM-1 AXIS:')
104   FORMAT('LXI  ',F7.1)
105   FORMAT('CM-1 SPACING OF TIC LABELS:')
106   FORMAT('CXL  ',F7.1)
107   FORMAT('AXES LENGTHS FOR CM-1 (FXL) & ABSORBANCE (LYT):')
108   FORMAT('FXL  ',F7.1)
109   FORMAT('LYT  ',F7.1)
110   FORMAT('AUTOSCALING: 0=NONE, 1=ALL, >1 = FILE SMN SCALE')
111   FORMAT('SMN  ',I5)
```

```
112   FORMAT('CM-1 LIMITS FOR AUTOSCALE:')
1130   FORMAT('XSP  ',I5)
1140   FORMAT('XEP  ',I5)
1141  FORMAT('DIGIT SIZE FOR ABSORBANCE LABELS; - KILLS LABELS')
1142  FORMAT('WTY  ',I5)
115   FORMAT('MARGIN (.01 INCHES) BETWEEN BASELINE & CM-1 AXIS')
1160   FORMAT('MNT  ',I5)
1170   FORMAT('ROTATE PLOT (0=NO, 1=YS)?')
1180   FORMAT('RTR  ',I5)
119   FORMAT('ORIGIN (INCHES) OF CM-1 (LXL) & ABSORBANCE (LYA)
     * AXES VS. ZPN:')
1200   FORMAT('LXL  ',F7.1)
1210   FORMAT('LYA  ',F7.1)
1240   FORMAT('INITIAL PEN # FOR SPECTRAL DATA:')
1250   FORMAT('PEK  ',I5)
126   FORMAT('ANGLE OF AXIS FOR CM-1 (SRT) & ABSORBANCE (RTN):')
1270   FORMAT('SRT  ',I5)
1280   FORMAT('RTN  ',I5)
129   FORMAT('ANGLE OF AXIS LABELS FOR CM-1 (FCD) & ABS (RTO):')
1310   FORMAT('FCD  ',F7.1)
1320   FORMAT('RTO  ',I5)
1330   FORMAT('ANGLE OF AXIS NAME FOR CM-1 (XSL) & ABS (YSL):')
1340   FORMAT('XSL  ',I5)
1350   FORMAT('YSL  ',I5)
1360   FORMAT('RATIO OF MINOR TO MAJOR TICS:')
1370   FORMAT('RTP  ',I5)
1380   FORMAT('PLOT TITLES (0=NO, 1=YES)?')
1390   FORMAT('VI2  ',I5)
1400   FORMAT('SPECTRUM PEN # INCREMENT FOR SUCCESSIVE PLOTS:')
1410   FORMAT('NSS  ',I5)
1420   FORMAT('# OF PLOTS:')
1430   FORMAT('QIT  ',I5)
1440   FORMAT('OVERLAP Y-AXES (0=NO, 1=YES) ?')
1450   FORMAT('OFN  ',I5)
1480   FORMAT('Y MARGIN BETWEEN PLOTS')
1490   FORMAT('VF4  ',F7.1)
      CALL EXIT
      END



!
C ------------------------------------------------------------
C "PMAC.FOR"
C
C CALLS: NONE
C ------------------------------------------------------------
C
      PROGRAM PMAC
      INTEGER LI(200),N(200),PGESIZ
      CHARACTER CHR(64)*1,OUT(64)*1,TEXT(60,64)*1,BL*1,IFILE*64
     $          ,TRIM*64,IFIL*64,ANYKEY*10
```

```
      DATA BL/' '/
C
C PROMPT FOR KEYBOARD INPUT:
C
      WRITE(2,1000)
      WRITE(2,900)
      READ(1,300) IFILE
      IFIL = TRIM( IFILE, 64 )
      OPEN(11,FILE= IFIL ,FORM='FORMATTED',STATUS='OLD')
      WRITE(2,400)
      READ(1,*) LPPAGE
      WRITE(2,500)
      READ(1,*) LSEP
      WRITE(2,600)
      READ(1,*) IUNPAK
      WRITE(2,700)
      READ(1,*) IPGSTP
      IF ( IPGSTP .NE. 1) IPGSTP = 0
      WRITE(2,1200)
      WRITE(2,1300)
      WRITE(2,1400)
      READ(1,*) NBLANK
      PGESIZ = NBLANK + LPPAGE
      IF (LSEP.LT.1.OR.LSEP.GT.LPPAGE) LSEP = 3
      IF (IUNPAK.NE.1) IUNPAK = 0
      LFLAG  = 0
      MARGIN = PGESIZ - LPPAGE
C
C READ 1ST LINE OF MACRO LISTING; THEN SKIP TO LINE 161:
C
            READ(11,100,END=8999) CHR
            L = 0
                                                        GO TO 161
C  INSERT "LSEP" BLANK LINES BETWEEN PREVIOUS & CURRENT MACRO:

C
21          LFLAG = (L - 1) * IUNPAK
            JMAX = LSEP + L
            IF (L+LSEP+1.GT.LPPAGE) JMAX = LPPAGE
             IF ( L + 1 . GT. JMAX )                    GO TO 61

      DO 51 J = L + 1, JMAX
      DO 41 I = 1, 64
41          TEXT(J,I) = BL
51          CONTINUE
C
C IF SUFFICIENT LINES HAVE ACCUMULATED, PRINT A PAGE OF TEXT.
C
61          IF (L+LSEP+1.GE.LPPAGE) THEN
                  DO 121 J = 1, L

                 DO 111 I = 1, 64
111                     OUT(I) = TEXT(J,I)
```

```
                        WRITE(10,200) OUT
121                     CONTINUE
                  DO 131 J = L + 1, PGESIZ
131                     WRITE(10,200) BL
                        L = 0
                        LFLAG = 0
                  IF (IPGSTP.EQ.1) THEN
                      WRITE(2,800)
                      READ(1,1100) ANYKEY
                      ENDIF
               ELSE
                        L = L + LSEP
               ENDIF
C
C  SAVE THE CURRENT MACRO HEADER LINE IN THE "TEXT" ARRAY:
C
161            L = L + 1
      DO 171 I=1,64
171            TEXT(L,I) = CHR(I)
C
C CONTINUE READING THE FILE UNTIL EITHER:
C   1) AN "END" STATEMENT IS FOUND,
C   2) "LPPAGE" LINES HAVE BEEN READ.
C
C FOR CASE 1, IGNORE SUBSEQUENT LINES UNTIL AN EXCLAMATION MARK
C IS FOUND.
C
181            READ(11,100,END=8999) CHR
               I1 = ICHAR(CHR(1))
               I2 = ICHAR(CHR(2))
               I3 = ICHAR(CHR(3))
               IF (I1.EQ.69. AND. I2.EQ.78. AND. I3.EQ.68) THEN
                        L = L + 1
                  DO 185 I= 1, 64
185                     TEXT(L,I) = CHR(I)
                        IGAP = 1
                        IF ( L. EQ. L )              GO TO 181
                        ENDIF
               IF (IGAP.EQ.1.AND.I1.NE.33)           GO TO 181
               IGAP = 0
C
C IF ONE EXCLAMATION  IS  FOUND, GO TO LINE 21.
C IF TWO EXCLAMATIONS ARE   "  , "   "  "   201 & PRINT OUTPUT.
C OTHERWISE, ADD THE CURRENT LINE TO THE "TEXT" ARRAY & THEN
C EITHER PRINT A FULL PAGE OR RETURN TO LINE 181.
C
               IF ( I1. EQ. 33. AND. I2. EQ. 33 )    GO TO 201
               IF ( I1. EQ. 33. AND. I2. NE. 33 )    GO TO 21
C
               L = L + 1
      DO 191 I= 1, 64
191            TEXT(L,I) = CHR(I)
C
```

```
C IF THE "IUNPAK = 1" OPTION HAS BEEN CHOSEN (I.E. LFLAG.NE.0)
C DON'T START PRINTING A MACRO IF IT BEGINS IN THE MIDDLE OF A
C PAGE AND EXTENDS BEYOND THE END OF THAT PAGE.  INSTEAD, PRINT
C THE PREVIOUS MACRO(S), RESHUFFLE THE INDICES OF "TEXT", AND
C START A FRESH PAGE.
C
201           IF (L.EQ.LPPAGE.AND.LFLAG.NE.0.AND.I2.NE.33) THEN
                  JMAX = LFLAG
              ELSE
                 JMAX = L
              ENDIF
C
C IF "LPPAGE" LINES HAVE BEEN READ OR IF "!!" IS ENCOUNTERED,
C TRANSFER DATA TO THE OUTPUT ARRAY AND PRINT IT.
C
              IF ( I2. EQ .33. OR. L. EQ. LPPAGE )  THEN
                    DO 221 J = 1, JMAX
                    DO 211 I = 1, 64
211                         OUT(I) = TEXT(J,I)
                            WRITE(10,200) OUT
221                         CONTINUE
                    DO 231 J = JMAX + 1, PGESIZ
231                         WRITE(10,200) BL
                               IF (IPGSTP.EQ.1) THEN
                                   WRITE(2,800)
                                   READ(1,1100) ANYKEY
                                   ENDIF
                 ENDIF
C
              IF (I2.EQ.33)                              GO TO 9999
C
C SKIP THE FOLLOWING "IF" UNLESS IUNPAK=1  ( I.E. LFLAG.NE.0),
C AND A PAGE HAS JUST BEEN PRINTED:
C
              IF (L.EQ.LPPAGE.AND.LFLAG.NE.0) THEN
                    DO 251 J = LFLAG+1, LPPAGE
                    DO 241 I = 1 , 64
                            JJ = J - LFLAG
                            TEXT(JJ,I) =  TEXT(J,I)
241                         TEXT(J,I)  =  BL
251                         CONTINUE
                            L = LPPAGE - LFLAG
                            LFLAG = 0
                            ENDIF
C
C SKIP THE FOLLOWING "IF" UNLESS IUNPAK=0 AND A PAGE HAS JUST
C BEEN PRINTED:
C
              IF (L.EQ.LPPAGE.AND.LFLAG.EQ.0) L = 0
                                                        GO TO 181
8999   PRINT *,'ERROR: EOF W/O TWO EXCLAMATION MARKS'
100    FORMAT(64A1)
200    FORMAT(1X,64A1)
```

```
300   FORMAT(A64)
400   FORMAT(1X,'# OF PRINTED LINES PER PAGE: ')
500   FORMAT(1X,'MINIMUM LINE SEPARATION BETWEEN MACROS: ')
600   FORMAT(1X,'START LONG MACROS ON NEW PAGE (0=NO, 1=YS)? ')
700   FORMAT(1X,'PAUSE AFTER EACH PAGE (0=NO, 1=YS)? ')
800   FORMAT(1X,'TYPE [CR] TO CONTINUE')
900   FORMAT('0','INPUT FILE NAME: ')
1000  FORMAT(1X,'*** THIS PROGRAM PRINTS MULTIPLE MACROS FROM
     $ A NICOS INPUT FILE ***')
1100  FORMAT(A10)
1200  FORMAT(1X,'# OF BLANK LINES NEEDED TO MATCH THE BLOCK OF
     $ PRINTED LINES WITH THE')
1300  FORMAT(1X,'PAGE SIZE OF THE PRINTER (DO NOT COUNT THE 6
     $ LINES THAT PRINTERS')
1400  FORMAT(1X,'AUTOMATICALLY SKIP ON EACH SIDE OF PAGE
     $ PERFORATIONS: ')
9999  STOP
      END



!
C ------------------------------------------------------------
C "SBFTYP.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACROS: AOB & SBS
C
C ------------------------------------------------------------
      PROGRAM SBFTYP
C
C "SBFTYP.FCP" IS CALLED BY MACROS "AOB" & "SBS" TO:
C
C 1) RECLASSIFY FTIR SCRATCH FILE "DFN" FROM %T TO 1-BEAM.
C 2) COMPUTE A MULTIPLIER FOR THE OUTPUT SCRATCH FILE.
C
      INTEGER IFSB(512),VI0
      INODE = IRVAL(13004,0)
      IBOUT = IRVAL(13761,0)
      VI0   = IRVAL(13762,0)
      ABSPT =  RVAL(13766,0)
      SBIPT =  RVAL(13770,0)
      NSECS = IRVAL(14001,0)
      NSD   = IRVAL(14006,0)
      IDFN  = IRVAL(14022,0)
      CALL IRTISK( IFSB, 512, NSECS * (IDFN + 1) + 87, INODE)
      IFSB(9) = -1
      IFSB(7) =  0
      CALL IWTISK( IFSB, 512, NSECS * (IDFN + 1) + 87, INODE)
      IF ( IBOUT. EQ. 0 )  FCD = SBIPT * 10 **( - ABSPT )
      IF ( IBOUT. EQ. 1 )  FCD = SBIPT * 10 **(   ABSPT )
```

```
      CALL RPUT( 14062, 0, FCD )
      CALL EXIT
      END



!
C ------------------------------------------------------------
C "SMT.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: SMT
C
C ------------------------------------------------------------
C
      PROGRAM SMT
C
C SMOOTH.FOR:  SMOOTHING PROGRAM FOR FTIR SCRATCH FILES.
C
C DATA PROCESSING SCHEME (ASSUME # OF COEFFICIENTS = 10):
C
C READ IDATA(1,512) > JDATA(  1,512)
C      IDATA(1,  9) >>>>>>>>>>>>>>>>>> SMOOTH(  1,  9)
C                   JDATA( 10,503) > SMOOTH( 10,503)
C                   JDATA(495,512) >>>>>>>>>>>>>>>>>>>>>>>
C >>>>>>>>>>>>>>>>>> JDATA(  1, 18)
C
C BEGIN LOOP:
C
C READ IDATA(1,512) > JDATA( 19,530)
C                   JDATA( 10, 18) > SMOOTH(504,512)
C                                    SMOOTH(  1,512) > WRITE
C                   JDATA( 19,521) > SMOOTH(  1,503)
C                   JDATA(513,530) >>>>>>>>>>>>>>>>>>>>>>>
C >>>>>>>>>>>>>>>>>> JDATA(  1, 18)
C END LOOP
C
C AFTER LAST LOOP:
C
C    IDATA(504,512) >>>>>>>>>>>>>>>>> SMOOTH(504,512)
C                                    SMOOTH(  1,512) >WRITE
C
      DIMENSION IDATA(512),C(100),JDATA(712)
      INTEGER SMOOTH(512),FILTYP
C
C READ FTIR PARAMETERS:
C
      INODE = IRVAL(13004,0)
      HWHM  =  RVAL(13766,0)
      NDPW  = IRVAL(14000,0)
```

```
      NSECS = IRVAL(14001,0)
      NTP   = IRVAL(14002,0) * 256
      ISFN  = IRVAL(14015,0)
      IDFN  = IRVAL(14022,0)
      WSMIN = IRVAL(14025,0)
      WSMAX = IRVAL(14026,0)
C ***************************************************************
C
C LOCATE SECTORS TO BE READ USING THE FOLLOWING INDEX:
C
      IDFSEC = IDFN * NSECS + 87
      ISFSEC = ISFN * NSECS + 87
C
C 1) COPY THE FILE STATUS BLOCK OF THE INPUT FILE TO THE OUTPUT
C    FILE.
C 2) IDENTIFY THE FILE AS A CM-1 FILE (FILTYP = 0) OR A
C    WAVELENGTH (FILTYP = 1) FILE.
C
      CALL IRTISK( IDATA, 512, ISFSEC + NSECS, INODE )
C
      IF ( IDATA(11) . EQ. 0 ) THEN
            FILTYP = 1
            WMIN   = IDATA(24)
            WMAX   = IDATA(25)
            PPW    = ( NTP / 2 - 1 ) / ( WMAX - WMIN )
         ELSE
            FILTYP = 0
            WMIN   = 0
            PPW    = 4.1482256 * NTP / 65536
         ENDIF
C
      CALL IWTISK( IDATA, 512, IDFSEC + NSECS, INODE )
C
C COMPUTE THE GAUSSIAN COEFFICIENTS CORRESPONDING TO THE GIVEN
C HALF-WIDTH AT HALF-MAXIMUM.
C
      HWHM  = HWHM * PPW
      B     =  0.470 / HWHM
      A     = -0.693 / (HWHM*HWHM)
C
C COMPUTE THE GAUSSIAN MULTIPLIERS; TRUNCATE THE GAUSSIAN AT
C SOME ARBITRARY POINT WHERE THE COEFFICIENTS BECOME
C NEGLIGIBLE.  THE CONVOLUTION INTEGRAL IS ALREADY NORMALIZED
C SINCE THE DATA POINT SPACING IS 1 UNIT.
C
      WRITE(2,1000)
1000  FORMAT('0','THE GAUSSIAN COEFFICIENTS ARE:')
      N    = 1
1     C(N) = B*2.7183**(A*(N-1)*(N-1))
      IF (C(N).LT.0.01*C(1).OR.N.GE.100)                GO TO 3
      WRITE(2,2000) N,C(N)
2000  FORMAT('0',I4,F10.3)
      N = N + 1
```

```
                                                              GO TO 1
3       NC = N
        NC1 = NC - 1
C
C COMPUTE INITIAL (IISEC) & FINAL (IFSEC) SECTORS:
C
        IF (WSMIN.GT.WSMAX) THEN
            TEMP  = WSMIN
            WSMIN = WSMAX
            WSMAX = TEMP
            ENDIF
C
        IIWORD = 1 + PPW * (WSMIN - WMIN)
        IISEC  = ( IIWORD - 1 ) / 512 + 1
        IFWORD = 1 + PPW * (WSMAX - WMIN)
        IFSEC  = ( IFWORD - 1 ) / 512 + 1
C
C PROCESS THE INITIAL SECTOR SEPARATELY SINCE IT MAY CONTAIN
C BLANKED POINTS.
C
                NSHIFT = 2 * NC1
                ISHIFT = 512 - NSHIFT
                MAXSMO = 512 - NC1
                CALL IRTISK( IDATA, 512, ISFSEC + IISEC, INODE )
                IPT = 1
        DO 100 J=1,512
                IF (IDATA(J).GE.-524287)                  GO TO 100
                IPT       = J + 1
                IDATA(J) = 0
100             JDATA(J) = IDATA(J)
                IF (IPT .LE. 1 )                          GO TO 115
        DO 110 M = 1, IPT - 1
110             SMOOTH(M) = JDATA(M)
115     DO 130 M = IPT, MAXSMO
                SMOOTH(M) = C(1) * JDATA(M)
                CSUM = C(1)
                IMAX = NC1
                IF (M .EQ. IPT)                           GO TO 125
                IF (M .LT. NC1 + IPT) IMAX = M - IPT
        DO 120 I = 1, IMAX
                IP1 = I + 1
                CSUM = CSUM + 2 * C(IP1)
120     SMOOTH(M) = SMOOTH(M)+C(IP1)*JDATA(M+I)+C(IP1)*JDATA(M-I)
125             SMOOTH(M) = SMOOTH(M) / CSUM
130             CONTINUE
        DO 140 I = 1, NSHIFT
140             JDATA(I) = JDATA(ISHIFT+I)
                 IF (IFSEC.EQ.IISEC)                      GO TO 320
C
C ***************************************************************
C
C BEGIN SMOOTHING LOOP:
C
```

```
      DO 300 K=IISEC+1,IFSEC
             IF(10*(K/10).EQ.K) PRINT *,'THE FIRST',K,'SECTORS
     $ HAVE BEEN PROCESSED THUS FAR'
             K1 = K - 1
             CALL IRTISK( IDATA, 512, ISFSEC + K, INODE )
      DO 150 I = 1, 512
             IF ( IDATA(I) .LT. -524287 ) IDATA(I) = 0
150           JDATA( I + NSHIFT ) = IDATA(I)
      DO 180 M = 1, NC1
             MM    = MAXSMO + M
             SMOOTH( MM ) = C(1) * JDATA( NC1 + M )
             NC1PM = NC1 + M
      DO 170 I = 1, NC1
             IP1   = I + 1
170        SMOOTH(MM) = SMOOTH(MM) + C(IP1) * JDATA( NC1PM + I )
     $                    +C(IP1) * JDATA( NC1PM - I )
180           CONTINUE
             CALL IWTISK( SMOOTH, 512, IDFSEC + K1, INODE)
      DO 250 M = 1, MAXSMO
             MM  = NSHIFT + M
             SMOOTH(M) = C(1) * JDATA( MM )
      DO 240 I = 1, NC1
             IP1 = I + 1
240           SMOOTH(M)  = SMOOTH(M) + C(IP1) * JDATA( MM + I )
     $          + C(IP1) * JDATA( MM - I )
250           CONTINUE
      DO 260 I = 1, NSHIFT
260           JDATA(I) = JDATA( 512 + I )
300           CONTINUE
C
C ***************************************************************
C
320   DO 350 I = 1, NC1
350           SMOOTH( MAXSMO + I ) = IDATA( MAXSMO + I )
             CALL IWTISK( SMOOTH, 512, IDFSEC + IFSEC, INODE )
      CALL EXIT
      END




!
C -------------------------------------------------------------
C "SORT.FOR"
C
C SUBROUTINE OF "AMAC.FOR"
C
C -------------------------------------------------------------
      SUBROUTINE SORT(NDATA,DATA,INDOUT)
      DIMENSION DATA(200),INDOUT(200)
C
C THIS SUBROUTINE SORTS "NDATA" DATA PTS FROM A "DATA" ARRAY
```

```
C IN ASCENDING ORDER.  "INDOUT" IS AN OUTPUT ARRAY OF INDICES
C THAT RELATES THE SORTED ORDERING TO THE UNSORTED ORDERING.
C
C INITIALIZE INDICES:
C
      DO 11 I = 1, NDATA
11          INDOUT(I) = I
            N1DATA = NDATA - 1
            NN = 0
C
C INCREMENT INDICES:
C
21          NN = NN + 1
            IF ( NN. GT . N1DATA )                          GO TO 101
31          N  = NN + 1
C
C COMPARE A PAIR OF POINTS:
C
41          IF ( DATA(N). LT . DATA(NN) )                   GO TO 61
51          N = N + 1
            IF ( N. GT . NDATA )                            GO TO 21
                                                            GO TO 41

C SWAP DATA ORDERING & INDEX ORDERING FOR A PAIR OF POINTS:
C
61          TMP         = DATA(N)
            DATA(N)     = DATA(NN)
            DATA(NN)    = TMP
C
            TMP         = INDOUT(N)
            INDOUT(N)   = INDOUT(NN)
            INDOUT(NN)  = TMP
                                                            GO TO 51
C
101         RETURN
            END



!
C ------------------------------------------------------------
C "SPLINE.FOR"
C
C SUBROUTINE OF "BASLIN.FOR" & "UVVIS.FOR"
C ------------------------------------------------------------
C SPLINE.FOR
C
C THIS SUBROUTINE COMPUTES COEFFICIENTS FOR CUBIC INTERPOLATION
C FORMULAS.
C ************************************************************
C
```

```
C  INPUT:
C        SPLOPT:  + VALUE: CUBIC INTERPOLATION.
C                 0      : SET ALL COEFFICIENTS TO 0.
C                 - VALUE: LINEAR INTERPOLATION.
C        NPTS = # OF DATA POINTS
C        XDATA(I),YDATA(I) = DATA ARRAYS
C        Y2DI,Y2DF = ESTIMATES OF THE 2ND DERIVATIVES AT THE
C                    INITIAL AND FINAL INTERPOLATION POINTS,
C                    RESPECTIVELY.
C
C  OUTPUT:
C        C(I,J) = ARRAY OF COEFFICIENTS (J = 1,2,3)
C
C *****************************************************************
C   THE COEFFICIENTS FOR THE ITH CUBIC EQN (COVERING RANGE I TO
C I+1) ARE GIVEN BY:
C
C   Y = C(I,3)*X**3 + C(I,2)*X**2 + C(I,1)*X + YDATA(I)
C
C    THE COEFFICIENTS ARE DEFINED SO THAT XDATA(I) CORRESPONDS
C TO X=0.
C *****************************************************************
C
      SUBROUTINE SPLINE(SPLOPT,NPTS,XDATA,YDATA,Y2DI,Y2DF,C)
      DIMENSION XDATA(10),YDATA(10),C(10,3),XUPDIF(2),YUPDIF(2),
     1          DIFRAT(2),R(10),CY2D(10,10),Y2D(10)
      INTEGER SPLOPT
C
            NDIM=NPTS-2
C
C      COMPUTE 2ND DERIVATIVES FROM AN ITERATIVE FORMULA
C DERIVED FROM BOUNDARY MATCHING CONDITIONS FOR 2ND DERIVATIVES.
C
            Y2D(1)=Y2DI
            Y2D(NPTS)=Y2DF
            MAXDIM=10
      DO 11 I=1,MAXDIM
            R(I)=0.0
      DO 11 J=1,3
11          C(I,J)=0.0
            IF (SPLOPT) 15,999,19
15    DO 17 I=1,MAXDIM
            DENOM=XDATA(I+1)-XDATA(I)
            IF (ABS(DENOM).LT.1.0E-6) GO TO 999
17          C(I,1)=(YDATA(I+1)-YDATA(I))/DENOM
            GO TO 999
19    DO 21 I=1,2
            XUPDIF(I)=XDATA(I+1)-XDATA(I)
            YUPDIF(I)=YDATA(I+1)-YDATA(I)
21          DIFRAT(I)=YUPDIF(I)/XUPDIF(I)
            R(1)=-XUPDIF(1)*Y2D(1)
      DO 51 I=1,NDIM
            IF (I.EQ.1) GO TO 31
```

```
              CY2D(I,I-1)=XUPDIF(1)
31            CY2D(I,I)=2*(XUPDIF(1)+XUPDIF(2))
              IF (I.EQ.NDIM) GO TO 41
              CY2D(I,I+1)=XUPDIF(2)
41            R(I)=6*(DIFRAT(2)-DIFRAT(1))+R(I)
              IF (I.EQ.NDIM) GO TO 51
              XUPDIF(1)=XUPDIF(2)
              XUPDIF(2)=XDATA(I+3)-XDATA(I+2)
              YUPDIF(2)=YDATA(I+3)-YDATA(I+2)
              DIFRAT(1)=DIFRAT(2)
51            DIFRAT(2)=YUPDIF(2)/XUPDIF(2)
              R(NDIM)=R(NDIM)-XUPDIF(2)*Y2D(NPTS)
C
C INVERT THE MATRIX OF 2ND-DERIVATIVE COEFFICIENTS:
C
              CALL MATINV(NDIM,CY2D)
C
C ***************************************************************
C COMPUTE 2ND DERIVATIVES FOR POINTS 2,3,...NPTS-1.
C
      DO 131 I=2,NPTS-1
              Y2D(I)=0.0
      DO 131 J=1,NDIM
131           Y2D(I)=Y2D(I)+CY2D(I-1,J)*R(J,1)
C
C ***************************************************************
C
C THE FOLLOWING EXPRESSIONS FOR THE CUBIC COEFFICIENTS ARE TRUE
C IN GENERAL BUT THE 2ND DERIVATIVES THAT APPEAR IN THESE
C EXPRESSIONS ARE DEPENDENT ON INPUT BOUNDARY CONDITIONS.
C
      DO 301 I=1,NPTS-1
      Q=      XDATA(I+1)-XDATA(I)
      C(I,3)= (Y2D(I+1)-Y2D(I))/(6*Q)
      C(I,2)= Y2D(I)/2
      C(I,1)= (YDATA(I+1)-YDATA(I)-Q*Q*(Y2D(I)/3+Y2D(I+1)/6))/Q
301   CONTINUE
999   RETURN
      END



!
C ---------------------------------------------------------
C "STICK.FOR"
C
C CALLS:  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: STK
C
C ---------------------------------------------------------
```

```
C
      PROGRAM STICK
C
C "STICK.FCP" GENERATES A STICK SPECTRUM USING INPUT
C ABSORBANCE DATA AT SEVERAL DISCRETE CM-1 VALUES.  IT IS RUN
C FROM MACRO "STK".  THE INPUT DATA MUST BE ENTERED INTO FILE
C "STICK.DAT" AS FOLLOWS:
C
C 1) ENTER THE # OF INPUT DATA POINTS (I4 FORMAT).
C
C 2) ENTER A PAIR OF (CM-1, ABSORBANCE) VALUES ON EACH NEW
C    LINE (2F7 FORMAT).
C
C 3) REPEAT STEPS 1 AND 2 FOR ANY ADDITIONAL SPECTRA.
C
      DIMENSION IDATA(512),F(50),A(50)
      OPEN(12,FILE='STICK.DAT',FORM='FORMATTED',STATUS='OLD')
C
C*****************************************************************
C READ FTIR PARAMETERS:
C
C   IDFN=DFN     NSECS~FSZ         ID=VI0 (DATA SET #)
C
      INODE=  IRVAL(13004,0)
      ID=     IRVAL(13762,0)
      NSECS=  IRVAL(14001,0)
      NPTS=   IRVAL(14002,0)*128
      IDFN=   IRVAL(14022,0)
C*****************************************************************
C
C LOCATE SECTORS TO BE READ USING THE FOLLOWING INDEX:
C
      IDFSEC = IDFN * NSECS + 88 - 1
C
C SET EXP=1 FOR THE TRANSMITTANCE FILE:
C
      CALL IRTISK( IDATA, 512, IDFSEC + NSECS, INODE )
      IDATA(6) = 1
      CALL IWTISK( IDATA, 512, IDFSEC + NSECS, INODE )
C
C WRITE TRANSMITTANCE = 1.0 FOR ALL DATA POINTS IN THE SCRATCH
C FILE TO CREATE A BASELINE (NOTE: DATA WORD = 262144 FOR T=1):
C
            PPWVN  = 4.148226 * NPTS / 32768
            MAXSEC = NPTS / 512
      DO 50 J = 1, 512
50          IDATA(J) = 262144
      DO 100 I = 1, MAXSEC
100   CALL IWTISK( IDATA, 512, IDFSEC + I, INODE )
C *****************************************************************
C
C READ INPUT DATA FROM FILE "STICK.DAT":
C
```

```
      DO 160 K = 1, ID
             READ(12,5000) NLINES
             PRINT *,NLINES
      DO 150 J = 1, NLINES
             READ(12,4000) F(J), A(J)
150          PRINT *,F(J), A(J)
160          CONTINUE
4000  FORMAT(2F7.2)
5000  FORMAT(I4)
C
C*****************************************************************
C
C SPECTRUM PROCESSING LOOP:
C
      DO 200 I = 1, NLINES
             IWORD  = 262144 * 10**( -A(I) )
             N      = 1 + PPWVN * F(I)
             ISEC   = N / 512 + 1
             NLOCAL = N - 512 * ( ISEC - 1 )
             CALL IRTISK( IDATA, 512, IDFSEC + ISEC, INODE )
             IDATA( NLOCAL ) = IWORD
200          CALL IWTISK( IDATA, 512, IDFSEC + ISEC, INODE )
C
C*****************************************************************
             CALL EXIT
             END




!
C ---------------------------------------------------------------
C "SUMSPC.FOR"
C
C CALLS: 1)   "FTPARM.FOR"
C        2)   FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: SUM
C
C ---------------------------------------------------------------
C
      PROGRAM SUMSPC
C
C THIS PROGRAM TAKES A LINEAR COMBINATION OF FTIR SCRATCH FILES
C ("IRFN" & "IDFN") IN THE CM-1 RANGE FROM "RFXF" TO "RLXF", AND
C SENDS THE RESULTS TO FILE "OFN"; I.E.
C
C FCR * (FILE IRFN) + FCD * (FILE IDFN) + ADDCON = FILE OFN
C
C WHERE "FCR", "FCD", & "ADDCON" ARE CONSTANTS.  THIS PROGRAM IS
C SIMILAR TO THE FTIR "ADD" OPERATION EXCEPT THAT:
C
```

```
C     1) THE OUTPUT MAY GO TO A NEW FILE.
C     2) ANY TYPE OF SPECTRA CAN BE ADDED.
C     3) AN ADDITIVE CONSTANT "ADDCON" CAN BE USED.
C
C BEFORE EXECUTING THIS PROGRAM, THE INPUT FILES MUST BE
C AUTOSCALED (C.F. MACRO "SU0") & THE MAXIMA MUST BE STORED IN
C FTIR PARAMETERS VF1 (YRMAX) & VF2 (YDMAX).
C
C WHEN ICHEXP=999 (FTIR PARAMETER 'SIZ') THE EXPONENT OF THE
C OUTPUT FILE IS SET AT 4; I.E. THE EXPONENT-DETERMINATION
C ALGORITHM IS SKIPPED.  THIS OPTION IS USED BY MACRO 'VCR'
C BECAUSE PIECEWISE ADDITION IS EMPLOYED.  NOTE THAT FOR 'VCR',
C THE OUTPUT FILE # MUST DIFFER FROM  THE INPUT FILE #'S
C BECAUSE OTHERWISE CHANGING THE INPUT FILE EXPONENT TO 4 WOULD
C ALTER THE ENTIRE FILE BEFORE THE FILE WAS FULLY PROCESSED.
C
C WHEN ICHEXP=9999 AND IDFN=OFN, THE EXPONENT OF OFN IS SET TO
C WHATEVER THE EXPONENT OF IDFN IS.
C
      INTEGER   OFN, OFSEC, OEXP
      DIMENSION IRDATA(512), IDDATA(512), IODATA(512)
C
C READ FTIR PARAMETERS AND INITIALIZE SECTOR INDICES:
C
            INODE  = IRVAL(13004,0)
            ICHEXP = IRVAL(13714,0)
            YRMAX  =  RVAL(13770,0)
            YDMAX  =  RVAL(13772,0)
            ADDCON =  RVAL(13774,0)
            NSECS  = IRVAL(14001,0)
            IDFN   = IRVAL(14022,0)
            OFN    = IRVAL(14023,0)
            IRFN   = IRVAL(14030,0)
            FCD    =  RVAL(14062,0)
            FCR    =  RVAL(14066,0)
            RFXF   =  RVAL(14135,0)
            RLXF   =  RVAL(14213,0)
C
            IRFSEC = IRFN * NSECS + 88 - 1
            IDFSEC = IDFN * NSECS + 88 - 1
            OFSEC  = OFN  * NSECS + 88 - 1
C
C READ THE FILE STATUS BLOCKS OF THE INPUT FILES TO:
C
C 1)  DETERMINE THE HENE CM-1.
C 1)  IDENTIFY SPECTRA AS 1-BEAM, TRANSMITTANCE, OR ABSORBANCE.
C 2)  DETERMINE THE EXPONENT AND # OF SCANS FOR THE SPECTRA.
C
            CALL IRTISK( IRDATA, 512, IRFSEC + NSECS, INODE )
            IREXP  = IRDATA(6)
            CALL IRTISK( IDDATA, 512, IDFSEC + NSECS, INODE )
            IDEXP  = IDDATA(6)
            ISNGLE = IDDATA(7)
```

```
            IHENE  = IDDATA(333)
C
C SET DATA BOUNDARY PARAMETERS:
C
      CALL FTPARM( IHENE, RFXF, RLXF, FRQMIN, FRQMAX, IISEC,
     1             IFSEC, INDXSP, INDXEP, PPWVN )
C
C FOR 1-BEAM SPECTRA, THE #'S OF SCANS OF THE 2 INPUT FILES ARE
C ADDED SINCE THE WEIGHTING FACTORS ARE ALREADY INCLUDED IN THE
C STORED DATA VALUES.  FOR OTHER SPECTRA, THE #'S OF SCANS ARE
C IRRELEVANT.
C
            IF (ISNGLE.EQ.0) IDDATA(3) = IRDATA(3) + IDDATA(3)
C
C USE THE MACRO AUTOSCALING RESULTS TO DETERMINE THE EXPONENT
C FOR THE OUTPUT FILE.  THEN SEND THE REVISED FILE STATUS BLOCK
C OF THE INPUT FILE "IRFN" TO THE OUTPUT FILE "OFN".
C
            NX     = -524288
            HX     =  524288.0
            RSCALE = 2 ** ( 19 - IREXP )
            DSCALE = 2 ** ( 19 - IDEXP )
            IF ( ICHEXP. EQ. 999 ) THEN
                 OEXP   = 4
               ELSEIF (ICHEXP.EQ.9999. AND. IDFN.EQ.OFN) THEN
                 OEXP   = IDEXP
               ELSE
                 OEXP   = 0
                 SUMMAX = (FCR*YRMAX +FCD*YDMAX +ADDCON) * HX
      DO 51      I = 1, 100
                 IF ( SUMMAX. LT. HX )              GO TO 81
                 SUMMAX = SUMMAX / 2
51               OEXP   = OEXP + 1
                 PRINT *,'EXPONENT ERROR IN SUM.FOR'
                 IF ( 2. EQ. 2 )                   GO TO 999
               ENDIF
81          IDDATA(6) = OEXP
            CALL IWTISK( IDDATA, 512, OFSEC + NSECS, INODE )
C
C READ THE 2 INPUT FILES, ADD THEM, AND SEND THE RESULTS TO THE
C OUTPUT FILE.  A BLANKED INPUT WORD IS CONVERTED TO ZERO
C WHENEVER THE CORRESPONDING WORD IN THE OTHER INPUT SPECTRUM IS
C NOT BLANKED.
C
            OSCALE = 2 ** ( 19 - OEXP )
      DO 201 M = IISEC, IFSEC
            CALL IRTISK( IRDATA, 512, IRFSEC + M, INODE )
            CALL IRTISK( IDDATA, 512, IDFSEC + M, INODE )
            CALL IRTISK( IODATA, 512, OFSEC  + M, INODE )
      DO 101 I = 1, 512
            KEEPR = 1
            KEEPD = 1
            IF ( IRDATA(I). EQ. NX )      PR = 0
```

```
            IF ( IDDATA(I). EQ. NX )  KEEPD = 0
            IF ( KEEPR. EQ. 0. AND. KEEPD. EQ. 0 )   GO TO 101
            IF ( M. EQ. IISEC. AND. I. LT. INDXSP )  GO TO 101
            IF ( M. EQ. IFSEC. AND. I. GT. INDXEP )  GO TO 101
            IODATA(I) = ( KEEPD * FCD * IDDATA(I) / DSCALE +
     1                  KEEPR*FCR*IRDATA(I)/RSCALE)*OSCALE+ADDCON
101         CONTINUE
201         CALL IWTISK( IODATA, 512, OFSEC + M , INODE )
999         CALL EXIT
            END



 !

C ------------------------------------------------------------
C "UVVIS.FOR"
C
C CALLS: 1)  "FSBTIT.FOR"
C        2)  "SPLINE.FOR" > "MATINV.FOR"
C        3)  FTIR SYSTEM SUBROUTINES
C
C CALLING MACRO: UVV
C
C ------------------------------------------------------------
C
      PROGRAM UVVIS
C
C "UVVIS.FCP" COPIES UV-VISIBLE DATA FROM A NICOS FILE INTO FTIR
C SCRATCH FILE "DFN".  TO RUN THIS PROGRAM, THE FOLLOWING
C PRELIMINARY STEPS MUST BE ACCOMPLISHED:
C
C     1) SEND SURVEY SPECTRA (474 PTS PER FILE) FROM THE PE
C        DIODE ARRAY SPECTROMETER TO THE HP150 USING THE
C        "SND.OY" PROGRAM ON THE PE DATA STATION, AND A LOGGING
C        FILE ON THE HP 50 OR ZENITH.
C
C     2) ARRANGE THE DATA IN COLUMNS USING PDAPAK.FOR ON THE
C        ZENITH OR HP150.
C
C     3) COPY THE ZENITH OR HP150 FILE TO THE NICOLET USING
C        XMODEM.
C
      INTEGER   TITLE(88)
      DIMENSION IDATA(512),WVL(474),WVLSPL(10),ASPL(10),
     $          CD(10,3),A(7,474)
      REAL      NI
      CHARACTER TERM*80, CONC*80, LET*2, LETSTR*80, LETNEW*3,
     $          FILNAM*80,TRIM*80
C*************************************************************
C
C INITIALIZE PARAMETERS:
C
```

```
            PRINT *,'UVVIS.FCP EXECUTION UNDERWAY'
            NPEPTS = 474
            IEXP   = 2
            NTP    = 2 * 512
            WVLII  = 900
            WVLFI  = 190
            WVLPPI = ( WVLII - WVLFI ) / ( NPEPTS - 1 )
            WVLPPO = ( WVLII - WVLFI ) / ( NTP - 1 )
      DO 11 I = 1, 4
11          WVLSPL(I) = I
C
C*****************************************************************
C READ FTIR PARAMETERS:
C
      INODE = IRVAL(13004,0)
      NSECS = IRVAL(14001,0)
      IDFN  = IRVAL(14022,0)
      IQIT  = IRVAL(14222,0)
C
C *****************************************************************
C
C READ DATA FROM INPUT FILE:
C
      OPEN( 12, FILE='UVVIS.DAT[UVV]', FORM='FORMATTED',
     $ STATUS='OLD' )
      IF (IQIT.EQ.1) THEN
            READ(12,100) WVL(1), A(1,1)
         ELSEIF (IQIT.EQ.2) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1)
         ELSEIF (IQIT.EQ.3) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1), A(3,1)
         ELSEIF (IQIT.EQ.4) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1), A(3,1), A(4,1)
         ELSEIF (IQIT.EQ.5) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1), A(3,1), A(4,1)
     $                  ,A(5,1)
         ELSEIF (IQIT.EQ.6) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1), A(3,1), A(4,1)
     $                  ,A(5,1), A(6,1)
         ELSEIF (IQIT.EQ.7) THEN
            READ(12,100) WVL(1), A(1,1), A(2,1), A(3,1), A(4,1)
     $                  ,A(5,1), A(6,1), A(7,1)
         ENDIF
C
      DO 101 I = 2, NPEPTS
      IF (IQIT.EQ.1) THEN
            READ(12,100) WVL(I), A(1,I)
         ELSEIF (IQIT.EQ.2) THEN
            READ(12,100) WVL(I), A(1,I), A(2,I)
         ELSEIF (IQIT.EQ.3) THEN
            READ(12,100) WVL(I), A(1,I), A(2,I), A(3,I)
         ELSEIF (IQIT.EQ.4) THEN
            READ(12,100) WVL(I), A(1,I), A(2,I), A(3,I), A(4,I)
```

```
            ELSEIF (IQIT.EQ.5) THEN
               READ(12,100) WVL(I), A(1,I), A(2,I), A(3,I), A(4,I)
     $                     ,A(5,I)
            ELSEIF (IQIT.EQ.6) THEN
               READ(12,100) WVL(I), A(1,I), A(2,I), A(3,I), A(4,I)
     $                     ,A(5,I), A(6,I)
            ELSEIF (IQIT.EQ.7) THEN
               READ(12,100) WVL(I), A(1,I), A(2,I), A(3,I), A(4,I)
     $                     ,A(5,I), A(6,I), A(7,I)
            ENDIF
101    CONTINUE
100    FORMAT( 1X, F6.2, 7(1X, F6.4) )
C
C*****************************************************************
C
       DO 301 J = 1, IQIT
              IFILE  = IDFN + J - 1
              PRINT *,'SENDING DATA TO FILE #: ',IFILE
              IDFSEC = IFILE * NSECS + 87
C
C SET OUTPUT FILE PARAMETERS:
C      1) 16 CM-1 RESOLUTION (DETERMINED BY "NTP")
C      2) 190 NM TO 900 NM
C      3) FILE EXPONENT = IEXP
C
       CALL IRTISK( IDATA, 512, IDFSEC + NSECS, INODE )
       IDATA(6)  = IEXP
       IDATA(7)  = -1
       IDATA(8)  = -1
       IDATA(9)  = -1
       IDATA(10) = 0
       IDATA(11) = 0
       IDATA(15) = 8
       IDATA(16) = 8
       IDATA(24) = 190
       IDATA(25) = 900
       CALL IWTISK( IDATA, 512, IDFSEC + NSECS, INODE )
C
C ***************************************************************
C
C CONVERT DATA TO NICOLET'S STYLE OF DATA STORAGE.  "NI" & "NO"
C ARE THE ORDERING INDICES FOR THE PERKIN-ELMER & NICOLET DATA,
C RESPECTIVELY.  THE # OF NICOLET DATA PTS IS ARBITRARILY SET
C AT NTP, REGARDLESS OF THE # OF PERKIN-ELMER PTS.
C INTERPOLATION IS USED TO CONVERT FROM THE INPUT DATA INTERVAL
C TO THE OUTPUT DATA INTERVAL.
C
              IDATA(1) = A(J, NPEPTS) * 2**( 19-IEXP )
       DO 201 NO = 2, NTP
              NI = 1 + ( ( 1 - NO ) * WVLPPO + 710 ) / WVLPPI
              IILOW    = INT(NI)
              REM      = NI - IILOW
C
```

```
                IF ( IILOW + 2 . LE. NPEPTS .AND. IILOW.GT.1 ) THEN
                  ASPL(1)  =  A(J, IILOW-1)
                  ASPL(2)  =  A(J, IILOW  )
                  ASPL(3)  =  A(J, IILOW+1)
                  ASPL(4)  =  A(J, IILOW+2)
                  CALL SPLINE(1,4,WVLSPL,ASPL, 0.0, 0.0, CD)
                  AO = A(J,IILOW) + CD(2,1)*REM +CD(2,2)*REM*REM
     $                 + CD(2,3)*REM*REM*REM
                ELSE
                  AO = A(J,IILOW)
     $                 + REM * ( A(J, IILOW+1) - A(J, IILOW) )
                ENDIF
C
                ISEC     = ( NO - 1 ) / 512
                I        = NO - 512 * ISEC
                IDATA(I) = AO * 2**( 19 - IEXP )
                ISEC     = IDFSEC + ISEC + 1
201             IF (I.EQ.512) CALL IWTISK(IDATA,512,ISEC,INODE)
301             CONTINUE
C
C*****************************************************************
999             CALL EXIT
                END
```

APPENDIX B

COMPUTER PROGRAMS FOR THE PERKIN-ELMER 7500 WORK STATION

The following software enables a block of UV-VIS spectral data files to be sent from the PE-7500 work station of the PE-3840 UV-VIS spectrometer to a logging file on an HP-150 or a Zenith-248 computer. Further transfer of data can be made from an HP-150 or Zenith-248 computer to the work station of the Nicolet Model 740 FT-IR spectrometer using XMODEM. Several benefits accrue from this procedure:

1. Data manipulations can be performed with IBM-compatible software (files created on the Zenith-248 can be used in this manner).

2. Plots can be produced with the GRAFIT software of the HP-150.

3. Plotting and other data manipulations can be performed using Nicolet's software. UV-VIS data can be loaded into Nicolet's FT-IR scratch files using the UVV macro described in Appendix A.

4. The speed of data manipulation can be greatly increased.

```
-------------------------------------------------------------
* "snd.oy"        (OBEY program)
*
* calls: "hp.ba"
* -----------------------------------------------------------
*
*      "snd.oy" sends a block of "*.sp" spectral data files from
* a floppy disk on the Perkin-Elmer 7500 to a logging file on an
* HP-150 or Zenith-248 via an intermediate PE-7500 scratch file
* "usr/uv/data/i.da".  All of the input files should be sent to
* one receiving file called "pda.dat" where they can later be
* re-separated into spectral files using "pdastk.for".
&11 *
* The input files must have:
*
*      1) a common file name of the form:      GEN###.sp
*         where GEN is a generic name consisting of 2 to 5
*         alphanumeric characters.
*
*      2) a data range from 190nm to 900nm
*
* Enter the # of files of input spectral data:
```

```
&enter a1
*
* Enter a data point reduction factor for RS-232 data
* transmission:
*      1 = send every spectral point.
*      2 = send every other spectral point.
*           etc.
*
&enter a10
*
* Enter all except the last 5 characters of the GENERIC input
* file name;  e.g. if the first file is named blank001.sp,
* enter: bla
&enter a2
*
* Enter the last 5 characters of the GENERIC input file name; the
* last 3 characters must be a 3-digit identification for the
* initial file in the set (ignore ".sp").  In the above example,
* one would enter:  nk001
&enter a3
*
* 1)    PUT THE DISK CONTAINING THE SPECTRAL DATA INTO DRIVE 0.
*       A SECOND DATA DISK MAY BE INSERTED INTO DRIVE 1 IF THE
*       FILE EXTENSIONS CONTINUE SEQUENTIALLY ONTO THIS SECOND
*       DISK.
* 2)    SET UP RECEIVING FILE "A:PDA.DAT" ON THE RECEIVING
*       COMPUTER.
* 3)    PRESS [ENTER] TO BEGIN DATA CONVERSION.  TO ABORT THIS
*       PROGRAM, PRESS [BREAK] AND THEN TYPE "VSAVE CLOSE".
*
do pause
do display off
calc v64=&a1
&def a17= "w4:i"
&def a6= "f0:"
&def a7= "f1:"
&def a8= a6
&for v2=1,v64
&def a4=  a2 + a3
&def a9=  a8 + a4 + ".sp"
do display on
&check a9
&error 160
&goto 162
&160
&def a8=a7
&def a9=a8 + a4 + ".sp"
&check a9
&error 161
&goto 162
&161 *FILE NOT FOUND*
&goto 11
&162 retrieve x &a9
```

```
calc v1=xstrt+0.001
calc v5=&a10*xdel
calc v3=int(xnpts/&a10+0.001)
calc v6=int(v3/20)
calc v7=int(-20*v6+v3)
vsave open new &a17
vsave &a17 v2
vsave &a17 a9
do display off
vsave &a17 v1
vsave &a17 v5
vsave &a17 v3
calc v10=xstrt+v5
&for v60=1,v6
calc v10=v10-v5
calc v11=x(v10)
calc v10=v10-v5
calc v12=x(v10)
calc v10=v10-v5
calc v13=x(v10)
calc v10=v10-v5
calc v14=x(v10)
calc v10=v10-v5
calc v15=x(v10)
calc v10=v10-v5
calc v16=x(v10)
calc v10=v10-v5
calc v17=x(v10)
calc v10=v10-v5
calc v18=x(v10)
calc v10=v10-v5
calc v19=x(v10)
calc v10=v10-v5
calc v20=x(v10)
calc v10=v10-v5
calc v21=x(v10)
calc v10=v10-v5
calc v22=x(v10)
calc v10=v10-v5
calc v23=x(v10)
calc v10=v10-v5
calc v24=x(v10)
calc v10=v10-v5
calc v25=x(v10)
calc v10=v10-v5
calc v26=x(v10)
calc v10=v10-v5
calc v27=x(v10)
calc v10=v10-v5
calc v28=x(v10)
calc v10=v10-v5
calc v29=x(v10)
calc v10=v10-v5
```

```
calc v30=x(v10)
vsave &a17 v11
vsave &a17 v12
vsave &a17 v13
vsave &a17 v14
vsave &a17 v15
vsave &a17 v16
vsave &a17 v17
vsave &a17 v18
vsave &a17 v19
vsave &a17 v20
vsave &a17 v21
vsave &a17 v22
vsave &a17 v23
vsave &a17 v24
vsave &a17 v25
vsave &a17 v26
vsave &a17 v27
vsave &a17 v28
vsave &a17 v29
vsave &a17 v30
&next v60
&for v8=1,v7
calc v10=v10-v5
calc v11=x(v10)
vsave &a17 v11
&next v8
vsave close
idris basic -r /usr/uv/data/hp.ba
&incr a3
&next v2
* ALL FILES CONVERTED
&11000 vsave close
* END
```

"hp.ba" (BASIC program)

Subroutine of "snd.oy"

```
$10 rem: "hp.ba" is a subroutine that reads spectral data from
20 rem: file "/usr/uv/data/i.da" on the Perkin-Elmer 7500, and
30 rem: sends it to a logging file on an HP-150 or a Zenith-248
40 rem: via the tty0 port.
50  dim s(10)
60  defwrd n
70 fi$="/usr/uv/data/i.da"
80 fo$="/dev/tty0"
90  open "i",# 5,fi$
```

```
100  open "o",# 6,fo$
110  input # 5,junk
120  input # 5,iter
130  input # 5,junk
140  input # 5,fhp$
150  input # 5,junk
160  input # 5,wvli
170  input # 5,junk
180  input # 5,wvlspa
190  input # 5,junk
200  input # 5,ndp
210 rdp= 1.0 *ndp
220 n= len (fhp$)
230 ofil$=fhp$
240 nxt1= asc ( right$ (fhp$, 3))
250 nxt2= asc ( right$ (fhp$, 2))
260 nxt3= asc ( right$ (fhp$,1))
270 rem: check that last 3 characters of file name are digits
280  if nxt1< 48 or nxt1> 57 goto 400
290  if nxt2< 48 or nxt2> 57 goto 400
300  if nxt3< 48 or nxt3> 57 goto 400
310 nxt= 100*nxt1+ 10*nxt2+nxt3- 5329+iter
320 ndig1=nxt/100
330 sbt=nxt- 100*ndig1
340 ndig2=sbt/ 10
350 ndig3=sbt-10*ndig2
360 ndig1=ndig1+ 48
370 ndig2=ndig2+ 48
380 ndig3=ndig3+ 48
390 ofil$=left$(fhp$,n- 3)+ chr$(ndig1)+ chr$(ndig2)+ chr$(ndig3)
400  print # 6,ofil$
410  print # 6,wvli
420  print # 6,wvlspa
430  print # 6,rdp
440 npline= 8
450 nfull=ndp/npline
460  for i=1  to nfull
470  for j=1  to npline
480  input # 5,junk,s(j)
490  next j
500print#6,using"-#.####";  1);s(2);s(3);s(4);s(5);s(6);s(7);s(8)
510  next i
520 nrem=ndp-npline*nfull
530  if nrem= 0 goto 610
540  for i=1  to nrem
550  input # 5,junk,s(i)
560  next i
570  for i=nrem+1  to npline
580 s(i)= 0
590  next i
600print#6,using"-#.####";s(1);s(2);s(3);s(4);s(5);s(6);s(7);s(8)
610  system
```

```
C ------------------------------------------------------------------
C "PDAPAK.FOR"
C
C Calls: none
C ------------------------------------------------------------------

      PROGRAM PDAPAK
C
C "PDAPAK.FOR" READS UV-VIS SURVEY SPECTRAL DATA (474 PTS / FILE)
C WHICH HAS BEEN SENT TO AN HP-150 OR ZENITH-248 LOGGING FILE
C NAMED "PDA.DAT" BY PERKIN-ELMER 7500 PROGRAM "SND.OY".
C     IT ORGANIZES THE DATA SO THAT EACH ROW CORRESPONDS TO A
C DIFFERENT WAVELENGTH, AND EACH COLUMN CORRESPONDS TO A
C DIFFERENT SPECTRUM.  EIGHT COLUMNS ARE WRITTEN TO OUTPUT FILE
C PDASTK.DAT (MAX OF 7 SPECTRA).
C
      DIMENSION Y(3324)
      CHARACTER FILNAM*10
      WRITE(*,400)
          OPEN(11,FILE='PDAPAK.DAT',STATUS='UNKNOWN',FORM=
     :         'FORMATTED')
          OPEN(10,FILE='PDA.DAT',STATUS='OLD',FORM='FORMATTED')
      DO 201 NFIL=1,7
          READ(10,100,END=301) FILNAM
          WRITE(*,600) FILNAM
          IF (NFIL.EQ.1) THEN
             WRITE(11,700) FILNAM
             WRITE(11,800)
             WRITE(11,900)
             WRITE(11,800)
             ENDIF
             N = NFIL
             READ( 10, 200 ) WVLI
             READ( 10, 200 ) WVLSPA
             READ(10,200) RDP
             WRITE(*,200) RDP
             NPLINE = 8
             NDP    = NINT(RDP)
             NLINES = NDP / NPLINE
             NREM   = NDP - NPLINE * NLINES
             IMAX   = NLINES
             IF ( NREM .EQ. 0 ) IMAX = NLINES - 1
             L = ( NFIL - 1 ) * NDP + 1
      DO 101 I = 0, IMAX
```

```
              READ(10, 200) Y(L), Y(L+1), Y(L+2), Y(L+3),Y(L+4),
     1                      Y(L+5),Y(L+6),Y(L+7)
101              L = L + 8
201              CONTINUE
301              N2 = 2 * NDP
                 N3 = 3 * NDP
                 N4 = 4 * NDP
                 N5 = 5 * NDP
                 N6 = 6 * NDP
                 W0 = WVLI + WVLSPA
       DO 311    J = 1, NDP
                 WVL = W0 - J * WVLSPA
              IF ( N .EQ. 1 ) THEN
                    WRITE(11,300) WVL,Y(J)
                 ELSEIF ( N .EQ. 2 ) THEN
                    WRITE(11,300) WVL, Y(J), Y(J+NDP)
                 ELSEIF (N.EQ.3) THEN
                    WRITE(11,300) WVL, Y(J), Y(J+NDP), Y(J+N2)
                 ELSEIF (N.EQ.4) THEN
                   WRITE(11,300)WVL,Y(J),Y(J+NDP),Y(J+N2),Y(J+N3)
                 ELSEIF (N.EQ.5) THEN
                 WRITE(11,300) WVL,Y(J),Y(J+NDP),Y(J+N2),Y(J+N3),
     $                         Y(J+N4)
                 ELSEIF (N.EQ.6) THEN
                 WRITE(11,300) WVL,Y(J),Y(J+NDP),Y(J+N2),Y(J+N3),
     $                         Y(J+N4),Y(J+N5)
                 ELSEIF (N.EQ.7) THEN
                 WRITE(11,300) WVL,Y(J),Y(J+NDP),Y(J+N2),Y(J+N3),
     $                         Y(J+N4),Y(J+N5),Y(J+N6)
                 ENDIF
311            CONTINUE
C
100           FORMAT(A10)
200           FORMAT(8F8.0)
300           FORMAT(1X,F6.2,7(1X,F6.4))
400           FORMAT(1X,'EXECUTION UNDERWAY')
500           FORMAT(1X,I3,' SPECTRA WERE PROCESSED')
600           FORMAT(1X,A10)
700           FORMAT('NAME OF FIRST FILE (COLUMN #2):  ',A10)
800           FORMAT(1X,' ')
900           FORMAT(4X,'NM     001    002    003    004',
     $                '    005    006    007')
C
9999          WRITE(*,500) N
              STOP
              END
```